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PROFESSOR: OK. Let's start. So last time, we started with kinetic theory. And we will focus for gas systems mostly. And the question that we would like to think about and answer somehow is the following. You start with a gas that is initially confined to one chamber. And you can calculate all of its thermodynamic properties. You open at time 0 a hole, allowing the gas to escape into a second initially empty chamber.

And after some time, the whole system will come to a new equilibrium position. It's a pretty reversible thing. You can do this experiment many, many times. And you will always get roughly the same amount of time for the situation to start from one equilibrium and reach another equilibrium. So how do we describe that? It's slightly beyond what we did in thermodynamics, because we want to go from one equilibrium state to another equilibrium state.

Now, we said, OK, we know the equations of motion that governs the particles that are described by this. So here we can say that we have, let's say, N particles. They have their own momenta and coordinates. And we know that these momenta and coordinates evolve in time, governed by some Hamiltonian, which is a function of all of these momenta and coordinates. OK? Fine.

How do we go from a situation which describes a whole bunch of things and coordinates that are changing with time to some microscopic description of macroscopic variables going from one equilibrium state to another? So our first attempt in that direction was to say, well, I could start with many, many, many examples of the same situation. Each one of them would correspond to a different trajectory of p 's and q 's.

And so what we can do is to construct some kind of an ensemble average, or

ensemble density, first, which is what we did. We can say that the very, very many examples of this situation that I can have will correspond to different points at some particular instant of time, occupying this $6N$ -dimensional phase space, out of which I can construct some kind of a density in phase space.

But then I realize that since each one of these trajectories is evolving according to this Hamiltonian, this density could potentially be a function of time. And we described the equation for the evolution of that density with time. And we could write it in this form-- $\dot{\rho}$ is the Poisson bracket of the Hamiltonian with ρ . And this Poisson bracket was defined as a sum over all of your coordinates. Oops. We had $\dot{\rho} = \sum_i \left(\frac{\partial \rho}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial H}{\partial q_i} \right)$ [? way. ?]

So there are essentially three N terms-- well, actually, six N terms, but three N pairs of terms in this sum. I can either use some index α running from one to three N , or indicate them as contributions of things that come from individual particles and then use this notation with three vectors. So this is essentially a combination of sum of three terms. OK?

So I hope that somehow this equation can describe the evolution that goes on over here. And ultimately, when I wait sufficiently long time, I will reach a situation where $\dot{\rho}$ does not change anymore. And I will find some density that is invariant on time. I'll call that ρ equilibrium. And so we saw that we could have our ρ equilibrium, which then should have zero Poisson bracket with H to be a function of H and any other conserved quantity. OK?

So in principle, we sort of thought of a way of describing how the system will evolve in equilibrium-- towards an equilibrium. And indeed, we will find that in statistical mechanics later on, we are going to rely heavily on these descriptions of equilibrium densities, which are governed by only the Hamiltonian. And if there are any other conserved quantities, typically there are not. So this is the general form that we'll ultimately be using a lot.

But we started with a description of evolution of these coordinates in time, which is time-reversible. And we hope to end up with a situation that is analogous to what we

describe thermodynamically, we describe something that goes to some particular state, and basically stays there, as far as the macroscopic description is concerned.

So did we somehow manage to just look at something else, which is this density, and achieve this transition from reversibility to irreversibility? And the answer is no. This equation-- also, if you find, indeed, a ρ that goes from here to here, you can set t to minus t and get a ρ that goes from back here to here. It has the same time-reversibility.

So somehow, we have to find another solution. And the solution that we will gradually build upon relies more on physics rather than the rigorous mathematical nature of this thing. Physically, we know that this happens. All of us have seen this. So somehow, we should be able to use physical approximation and assumptions that are compatible with what is observed. And if, during that, we have to sort of make mathematical approximations, so be it. In fact, we have to make mathematical approximations, because otherwise, there is this very strong reversibility condition.

So let's see how we are about to proceed, thinking more in terms of physics. Now, the information that I have over here, either in this description of ensemble or in this description in terms of trajectories, is just enormous. I can't think of any physical process which would need to keep track of the joined positions of coordinates and momenta of 10^{23} particles, and know them with infinite precision, et cetera.

Things that I make observations with and I say, we see this, well, what do we see? We see that something has some kind of a density over here. It has some kind of pressure. Maybe there is, in the middle of this process, some flow of gas particles. We can talk about the velocity of those things.

And let's say even when we are sort of being very non-equilibrium and thinking about velocity of those particles going from one side to the other side, we really don't care which particle among the 10^{23} is at some instant of time contributing to the velocity of the gas that is swishing past.

So clearly, any physical observable that we make is something that does not require

all of those degrees of freedom. So let's just construct some of those things that we may find useful and see how we would describe evolutions of them.

I mean, the most useful thing, indeed, is the density. So what I could do is I can actually construct a one-particle density. So I want to look at some position in space at some time t and ask whether or not there are particles there. I don't care which one of the particles. Actually, let's put in a little bit more information; also, keep track of whether, at some instant of time, I see at this location particles. And these particles, I will also ask which direction they are moving. Maybe I'm also going to think about the case where, in the intermediate, I am flowing from one side to another. And keeping track of both of these is important.

I said I don't care which one of these particles is contributing. So that means that I have to sum over all particles and ask whether or not, at time t , there is a particle at location q with momentum p . So these delta functions are supposed to enforce that. And again, I'm not thinking about an individual trajectory, because I think, more or less, all of the trajectories are going to behave the same way. And so what I will do is I take an ensemble average of this quantity. OK?

So what does that mean? To do an ensemble average, we said I have to integrate the density function, ρ , which depends on all of the coordinates. So I have coordinate for particle one, coordinate-- particle and momentum, particle and momentum for particle two, for particle three, all the way to particle number N . And this is something that depends on time. That's where the time dependence comes from.

And again, let's think about the time dependence where 0 is you lift the partition and you allow things to go from one to the other. So there is a non-equilibrium process that you are following. What I need to do is I have to multiply this density with the function that I have to consider the average.

Well, the function being a delta function, it's very nice. The first term in the sum, we'll set simply q_1 equals to q . And it will set p_1 equals to p when I do the integration over p_1 and q_1 . But then I'm left to have to do the integration over

particle two, particle three, particle four, and so forth. OK?

But this is only the first term in the sum. Then I have to write the sum for particle number two, particle number three, et cetera. But all of the particles, as far as I'm concerned, are behaving the same way. So I just need to multiply this by a factor of N .

Now, this is something that actually we encountered before. Recall that this ρ is a joint probability distribution. It's a joint probability distribution of all N particles, their locations, and momentum. And we gave a name to taking a joint probability density function, which this is, and integrating over some subset of variables. The answer is an unconditional probability distribution. So essentially, the end of this story is if I integrate over coordinates of two all the way to N , I will get an unconditional result pertaining to the first set of coordinate.

So this is the same thing up to a factor of N -- the unconditional probability that I will call ρ one. Actually, I should have called this f_1 . So this is something that is defined to be the one particle density. I don't know why this name stuck to it, because this one, that is up to a factor of N different from it, is our usual unconditional probability for one particle. So this is ρ of p_1 being p , q_1 being q at time. OK?

So essentially, what I've said is I have a joint probability. I'm really interested in one of the particles, so I just integrate over all the others. And this is kind of not very elegant, but that's somehow the way that it has appeared in the literature. The entity that I have on the right is the properly normalized probability. Once I multiply by N , it's a quantity this is called f_1 . And it's called a density and used very much in the literature. OK?

And that's the thing that I think will be useful. Essentially, all of the things that I know about observations of a system, such as its density, its velocity, et cetera, I should be able to get from this.

Sometimes we need a little bit more information, so I allow for the possibility that I

may also need to focus on a two-particle density, where I keep information pertaining to two particles at time t and I integrate over everybody else that I'm not interested.

So I introduce an integration over coordinates number two-- sorry, number three all the way to N to not have to repeat this combination all the time. The $6N$ -dimensional phase space for particle i I will indicate by dV_i . So I take the full N particle density, if you like, integrate over everybody except 2. And up to a normalization of $N(N-1)$, this is called a two-particle density.

And again, absent this normalization, this is simply the unconditional probability that I would construct out of this joint probability [INAUDIBLE].

And just for some mathematical purposes, the generalization of this to S particles, we will call f_S . So this depends on p_1 through q_S at time t . And this is going to be N factorial divided by $(N-S)$ factorial in general. And they join the unconditional probability that depends on S coordinates p_1 through q_S at time t . OK?

You'll see why I need these higher ones although, in reality, all my interest is on this first one, because practically everything that I need to know about this initial experiment that I set up and how a gas expands I should be able to extract from this one-particle density. OK? So how do I calculate this?

Well, what I would need to do is to look at the time variation of f_S with t to calculate the time dependence of any one of these quantities. Ultimately, I want to have an equation for df_1/dt . But let's write the general one.

So the general one is up to, again, this N factorial, $(N-s)$ factorial and integral over coordinates that I'm not interested, of $d\rho/dt$. OK? So I just take the time derivative inside the integral, because I know how $d\rho/dt$ evolves. And so this is going to be simply the Poisson bracket of H and ρ . And I would proceed from there.

Actually, to proceed further and in order to be able to say things that are related to physics, I need to say something about the Hamiltonian. I can't do so in the most

general case. So let's write the kind of Hamiltonian that we are interested and describes the gas-- so the Hamiltonian for the gas in this room.

One term is simply the kinetic energy. Another term is that gas particles are confined by some potential. The potential could be as easy as the walls of this room. Or it could be some more general potential that could include gravity, whatever else you want. So let's include that possibility.

So these are so-called one-body terms, because they pertain to the coordinates of one particle. And then there are two-body terms. So for example, I could look at all pairs of particles. Let's say $i \neq j$ to avoid self-interaction. V of q_i minus q_j . So certainly, two particles in this gas in this room, when they get close enough, they certainly can pass through each other. They each have a size. But even when they are a few times their sizes, they start to feel some interaction, which causes them to collide. Yes.

AUDIENCE: The whole series of arguments that we're developing, do these only hold for time-independent potentials?

PROFESSOR: Yes. Although, it is not that difficult to sort of go through all of these arguments and see where the corresponding modifications are going to be. But certainly, the very first thing that we are using, which is this one, we kind of implicitly assume the time-independent Hamiltonian. So you have to start changing things from that point. OK?

So in principle, you could have three-body and higher body terms. But essentially, most of the relevant physics is captured by this. Even for things like plasmas, this would be a reasonably good approximation, with the Coulomb interaction appearing here. OK?

Now, what I note is that what I have to calculate over here is a Poisson bracket. And then I have to integrate that Poisson bracket. Poisson bracket involves a whole bunch of derivatives over all set of quantities. And I realize that when I'm integrating over derivatives, there are simplifications that can take place, such as integration by parts. But that only will take place when the derivative is one of the variables that is

being integrated.

Now, this whole process has separated out arguments of ρ , as far as this expression is concerned, into two sets-- one set, or the set that is appearing out here, the first s ones that don't undergo the integration, and then the remainder that do undergo the integration.

So this is going to be relevant when we do our manipulations. And therefore, it is useful to rewrite this Hamiltonian in terms of three entities. The first one that I call $H_{\text{sub } s}$ -- so if you like, this is an end particle Hamiltonian. I can write an $H_{\text{sub } s}$, which is just exactly the same thing, except that it applies to coordinates that I'm not integrating over. And to sort of make a distinction, I will label them by N . And it includes the interaction among those particles.

And I can similarly write something that pertains to coordinates that I am integrating over. I will label them by j and k . So this is $s + 1$ to N , p_j^2 over $2m$ plus U of q_j plus $1/2$ sum over j and k , V of q_j minus q_k . OK?

So everything that involves one set of coordinates, everything that involves the other set of coordinates. So what is left are terms that [ρ copy ?] one set of coordinates to another. So N running from 1 to s , j running from $s + 1$ to N , V between q_m and q_j . OK?

So let me rewrite this equation rather than in terms of-- f in terms of the probabilities' ρ s. So the difference only is that I don't have to include this factor out front. So I have dV . I have the $d\rho$ by dt , which is the commutator of H with ρ , which I have been writing as H_s plus H_N minus s . I'm changing the way I write s . Sorry. Plus H' and ρ . OK?

So there is a bit of mathematics to be performed to analyze this. There are three terms that I will label a , b , and c , which are the three Poisson brackets that I have to evaluate. So the contribution that I call a is the integral over coordinates $s + 1$ to N , of the Poisson bracket of H_s with ρ . Now, the Poisson bracket is given up here. It is a sum that involves N terms over all N particles.

But since, if I'm evaluating it for H_s and H_s will only give nonzero derivatives with respect to the coordinates that are present in it, this sum of N terms actually becomes simply a sum of small N terms. So I will get a sum over N running from 1 to s . These are the only terms. And I will get the things that I have for $d\rho$ by dp_N -- sorry, ρ by dq_N , dH_s by dp_N minus $d\rho$ by dp_N , dH_s by dq_N . OK?

Did I make a mistake?

AUDIENCE: Isn't it the Poisson bracket of ρ and H , not H and ρ ?

PROFESSOR: ρ . Oh, yes. So I have to put a minus sign here. Right. Good. Thank you. OK.

Now, note that these derivatives and operations that involve H_s involve coordinates that are not appearing in the integration process. So I can take these entities that do not depend on variables that are part of the integration outside the integration, which means that I can then write the result as being an exchange of the order of the Poisson bracket and the integration.

So I would essentially have the integration only appear here, which is the same thing as H_s and ρ_s . This should be ρ_s . This is the definition of ρ_s , which is the same thing as ρ . OK.

What does it mean physically? So it's actually much easier to tell you what it means physically than to do the math. So what we saw was happening was that if I have a Hamiltonian that describes N particles, then for that Hamiltonian, the corresponding density satisfies this Liouville equation. $D\rho/dt$ is $HN\rho$. And this was a consequence of this divergence-less character of the flow that we have in this space, that the equations that we write down over here for \dot{p} and \dot{q} in terms of H had this character that the divergence was 0. OK?

Now, this is true if I have any number of particles. So if I focus simply on s of the particles, and they are governed by this Hamiltonian, and I don't have anything else in the universe, as far as this Hamiltonian is concerned, I should have the analog of a Liouville equation. So the term that I have obtained over there from this first term is simply stating that $d\rho_s/dt$, if there was no other interaction with anybody

else, would simply satisfy the corresponding Liouville equation for s particles.

And because of that, we also expect and anticipate-- and I'll show that mathematically-- that the next term in the series, that is the Poisson bracket of N minus s and ρ , should be 0, because as far as this s particles that I'm focusing on and how they evolve, they really don't care about what all the other particles are doing if they are not [INAUDIBLE]. So anything interesting should ultimately come from this third term. But let's actually go and do the calculation for the second term to show that this anticipation that the answer should be 0 does hold up and why.

So for the second term, I need to calculate a similar Poisson bracket, except that this second Poisson bracket involves H of N minus s . And H of N minus s , when I put in the full sum, will only get contribution from terms that start from s plus 1.

So the same way that that started from N , this contribution starts from s plus 1 to N . And actually, I can just write the whole thing as above, $d\rho$ by dq_j dotted by dH_{N-s} minus s by dp_j , plus $d\rho$ by-- no, this is the ρ . $d\rho$ by dp_j dotted by dH_{N-s} by dq_j .

So now I have a totally different situation from the previous case, because the previous case, the derivatives were over things I was not integrating. I could take outside the integral. Now all of the derivatives involve things that I'm integrating over. Now, when that happens, then you do integration by parts. So what you do is you take ρ outside and let the derivative act on everything else. OK?

So what do we end up with if we do integration by parts? I will get surface terms. Surface terms are essentially ρ -evaluated when the coordinates are at infinity or at the edge of your space, where ρ is 0. So there is no surface term. There is an overall change in sign, so I will get a product i running from s plus 1 to N , dV_i . Now the ρ comes outside. And the derivative acts on everything that is left.

So the first term will give me a second derivative of H_{N-s} , with respect to p , with respect to q . And the second term will be essentially the opposite way of doing the derivative. And these two are, of course, the same. And the answer is 0. OK?

So we do expect that the evolution of all the other particles should not affect the subset that we are looking at. And that's worn out also. So the only thing that potentially will be relevant and exciting is the last term, number c. So let's take a look at that.

So here, I have to do an integration over variables that I am not interested. And then I need now, however, to do a full Poisson bracket of a whole bunch of terms, because now the terms that I'm looking at have coordinates from both sets. So I have to be a little bit careful. So let me just make sure that I follow the notes that I have here and don't make mistakes. OK.

So this H' involves two sums. So I will write the first sum, N running from 1 to s . And then I have the second sum, j running from $s + 1$ to N . What do I need? I need the-- OK. Let's do it the following way.

So what I have to do for the Poisson bracket is a sum that involves all coordinates. So let's just write this whole expression. But first, for coordinates 1 through s . So I have a sum N running from 1 to s . And then I will write the term that corresponds to coordinates $s + 1$ to m .

For the first set of coordinates, what do I have? I have $d\rho$ by dq_n . And then I have dH' by dp_n . So I didn't write H' explicitly. I'm just breaking the sum over here. And then I have sum j running from $s + 1$ to N , $d\rho$ by dq_j times dH' by dp_j . And again, my H' is this entity over here that [? copies ?] coordinates from both sets. OK.

First thing is I claim that one of these two sets of sums is 0. You tell me which.

AUDIENCE: The first.

PROFESSOR: Why first?

AUDIENCE: Because H' is independent of p [? dot. ?]

PROFESSOR: That's true. OK. That's very good. And then it sort of brings up a very important

question, which is, I forgot to write two more terms.

[LAUGHTER]

Running to s of $d\rho$ by dp_n , dH prime by dq_n minus $\sum_{j=1}^N d\rho$ by dp_j dot dH prime by dq_j . So indeed, both answers now were correct. Somebody said that the first term is a 0, because H prime does not depend on p_n . And somebody over here said that this term is 0. And maybe they can explain why.

AUDIENCE: [INAUDIBLE].

PROFESSOR: Same reason as up here. That is, I can do integration by parts.

AUDIENCE: [INAUDIBLE].

PROFESSOR: To get rid of this term plus this term together. So it's actually by itself is not 0. But if I do integration by parts, I will have-- actually, even by itself, it is 0, because I would have d by dq_j , d by p_j , H prime. And H prime, you cannot have a double derivative p_j . So each one of them, actually, by itself is 0. But in general, they would also cancel each other through their single process. Yes.

AUDIENCE: Do you have the sign of $[dH]$ of $[H$ prime?]

PROFESSOR: Did I have the sign incorrect? Yes. Because for some reason or other, I keep reading from here, which is ρ and H . So let's do this. OK?

AUDIENCE: Excuse me.

PROFESSOR: Yes?

AUDIENCE: [INAUDIBLE].

PROFESSOR: OK. Yes, it is different. Yes. So what I said, if I had a more general Hamiltonian that also depended on momentum, then this term would, by itself not 0, but would cancel, be the corresponding term from here. But the way that I have for H prime, indeed, each term by itself would be 0. OK. So hopefully-- then what do we have?

So actually, let's keep the sign correct and do this, because I need this right sign for the one term that is preserved. So what does that say? It is a sum, n running from 1 to s . OK? I have dH prime by dq_n .

And I have this integration. I have the integration i running from s plus 1 to N dV of i . I have $d\rho$ by dp_n dot product with dH prime by dq_N . dH prime by dq_n I can calculate from here, is a sum over terms j running from s plus 1 to N of V of q_n minus q_j . All right.

AUDIENCE: Question.

PROFESSOR: Yes.

AUDIENCE: Why aren't you differentiating [$? me ?$] if you're differentiating H prime?

PROFESSOR: d by dq_j . All right?

AUDIENCE: Where is the q_n ?

PROFESSOR: d by dq_n . Thank you. Right. Because always, p_n of q_n would go together. Thank you. OK. All right.

So we have to slog through these derivations. And then I'll give you the physical meaning. So I can rearrange this. Let's see what's happening here. I have here a sum over particles that are not listed on the left-hand side. So when I wrote this $d\rho$ by dt , I had listed coordinates going from p_1 through q_s that were s coordinates that were listed. If you like, you can think of them as s particles.

Now, this sum involves the remaining particles. What is this? Up to a sign. This is the force that is exerted by particle j from the list of particles that I'm not interested on one of the particles on the list that I am interested. OK?

Now, I expect that at the end of the day, all of the particles that I am not interested I can treat equivalently, like everything that we had before, like how I got this factor of N or N minus 1 over there. I expect that all of these will give me the same result, which is proportional to the number of these particles, which is N minus s . OK? And

then I can focus on just one of the terms in this sum. Let's say the term that corresponds to j , being $s + 1$.

Now, having done that, I have to be careful. I can do separately the integration over the volume of this one coordinate that I'm keeping, V of $s + 1$. And what do I have here? I have the force that exerted on particle number N by the particle that is labelled $s + 1$.

And this force is dot producted with a gradient along the momentum in direction of particle N of its density. Actually, this is the density of all particles. This is the ρ that corresponds to the joint. But I had here $s + 1$ integrations. One of them I wrote down explicitly. All the others I do over here. Of the density.

So basically, I change the order of the derivative and the integrations over the variables not involved in the remainder. And the reason I did that, of course, is that then this is my ρ_{s+1} . OK? So what we have at the end of the day is that if I take the time variation of an s particle density, I will get one term that I expected, which is if those s particles were interacting only with themselves, I would write the Liouville equation that would be appropriate to them.

But because of the collisions that I can have with particles that are not over here, suddenly, the momenta that I'm looking at could change. And because of that, I have a correction term here that really describes the collisions. It says here that these s particles were following the trajectory that was governed by the Hamiltonian that was peculiar to the s particles.

But suddenly, one of them had a collision with somebody else. So which one of them? Well, any one of them. So I could get a contribution from any one of the s particles that is listed over here, having a collision with somebody else.

How do I describe the effect of that? I have to do an integration over where this new particle that I am colliding with could be. I have to specify both where the particle is that I am colliding with, as well as its momentum. So that's this. Then I need to know the force that this particle is exerting on me. So that's the V of $q_{s+1} - q_N$

divided by dq_N . This is the force that is exerted by this particle that I don't see on myself.

Then I have to multiply this, or a dot product of this, with d by dp_N , because what happens in the process, because of this force, the momentum of the N particle is changing. The variation of that is captured through looking at the density that has all of these particles in addition to this new particle that I am colliding with.

But, of course, I am not really interested in the coordinate of this new particle, so I integrate over it. There are $N - s$ such particles. So I really have to put a factor of $N - s$ here for all of potential collisions. And so that's the equation.

Again, it is more common, rather than to write the equation for ρ , to write the equation for f . And the f 's and the ρ 's where simply related by these factors of N factorial over $N - s$ factorial. And the outcome of that is that the equation for f simply does not have this additional factor of $N - s$, because that disappears in the ratio of ρ of $s + 1$ and ρ of s .

And it becomes a sum over N running from 1 to s . Integral over coordinates and momenta of a particle $s + 1$. The force exerted by particle $s + 1$ on particle N used to vary the momentum of the N particle. And the whole thing would depend on the density that includes, in addition to the s particles that I had before, the new particle that I am colliding with. OK?

So there is a set of equations that relates the different densities and how they evolve in time. The evolution of f_1 , which is the thing that I am interested, will have, on the right-hand side, something that involves f_2 . The evolution of f_2 will involve f_3 . And this whole thing is called a BBGKY hierarchy, after people whose names I have in the notes.

[SOFT LAUGHTER]

But again, what have we learned beyond what we had in the original case? And originally, we had an equation that was governing a function in $6N$ -dimensional

space, which we really don't need. So we tried our best to avoid that. We said that all of the physics is in one particle, maybe two particle densities. Let's calculate the evolution of one-particle and two-particle densities.

Maybe they will tell us about this non-equilibrium situation that we set up. But we see that the time evolution of the first particle density requires two-particle density. Two-particle density requires three-particle densities. So we sort of made this ladder, which ultimately will [? terminate ?] at the Nth particle densities. And so we have not really gained much. So we have to now look at these equations a little bit more and try to inject more physics.

So let's write down the first two terms explicitly. So what I will do is I will take this Poisson bracket of H and f, to the left-hand side, and use the Hamiltonian that we have over here to write the terms. So the equation that we have for f_1 -- and I'm going to write it as a whole bunch of derivatives acting on f_1 . f_1 is a function of p_1 q_1 t .

And essentially, what Liouville's theorem says is that as you move along the trajectory, the total derivative is 0, because the expansion of the flows is incompressible. So what does that mean? It means that d by dt , which is this argument, plus \dot{q}_1 times d by dq_1 plus \dot{p}_1 times d by dp_1 . So here, I should write \dot{p}_1 and \dot{q}_1 . In the absence of everything else is 0.

Then, of course, for \dot{q}_1 , we use the momentum that we would get out of this. \dot{q}_1 is momentum divided by mass. So that's the velocity. And \dot{p}_1 , changing momentum, is the force, is minus dH by dq_1 . So this is minus d of this one particle potential divided by dq_1 dotted by [? h ?] p_1 .

So if you were asked to think about one particle in a box, then you know its equation of motion. If you have many, many realizations of that particle in a box, you can construct a density. Each one of the elements of the trajectory, you know how they evolve according to [? Newton's ?] equation.

And you can see how the density would evolve. It would evolve according to this. I

would have said, equal to 0. But I can't set it to 0 if I'm really thinking about a gas, because my particle can come and collide with a second particle in the gas. The second particle can be anywhere. And what it will do is that it will exert a force, which would be like this, on particle one. And this force will change the momentum. So my variation of the momentum will not come only from the external force, but also from the force that is coming from some other particle in the medium.

So that's where this d by dp really gets not only the external force but also the force from somebody else. But then I need to know where this other particle is, given that I know where my first particle is. So I have to include here a two-particle density which depends on p_1 as well as q_2 at time t . OK. Fine.

Now you say, OK, let's write down-- I need to know f_2 . Let's write down the equation for f_2 . So I will write it more rapidly. I have p_1 over m , d by dq_1 . I have p_2 over m , d by dq_2 . I will have dU by dq_1 , d by dp_1 . I will have dU by dq_2 , d by dp_2 . I will have also a term from the collision between q_1 and q_2 .

And once it will change the momentum of the first particle, but it will change the momentum of the second particle in the opposite direction. So I will put the two of them together. So this is all of the terms that I would get from H_2 , Poisson bracket with density acting on the two-particle density. And the answer would be 0 if the two particles were the only thing in the box.

But there's also other particles. So there can be interactions and collisions with a third particle. And for that, I would need to know, let's actually try to simplify notation. This is the force that is exerted from two to one. So I will have here the force from three to one dotted by d by dp_1 . Right. And the force that is exerted from three to two dotted by d by dp_2 acting on a three-particle density that involves everything up to three.

And now let's write the third one.

[LAUGHTER]

So that, I will leave to next lecture. But anyway, so this is the structure. Now, this is the point at which we would like to inject some physics into the problem.

So what we are going to do is to estimate the various terms that are appearing in this equation to see whether there is some approximation that we can make to make the equations more treatable and handle-able. All right?

So let's try to look at the case of a gas-- let's say the gas in this room. A typical thing that is happening in the particles of the gas in this room is that they are zipping around. Their velocity is of the order-- again, just order of magnitude, hundreds of meters per second. OK?

So we are going to, again, be very sort of limited in what we are trying to describe. There is this experiment. Gas expands into a chamber. In room temperature, typical velocities are of this order.

Now we are going to use that to estimate the magnitude of the various terms that are appearing in this equation. Now, the whole thing about this equation is variation with time. So the entity that we are looking at in all of these brackets is this d by dt , which means that the various terms in this differential equation, apart from d by dt , have to have dimensions of inverse time. So we are going to try to characterize what those inverse times are.

So what are the typical magnitudes of various terms? If I look at the first equation, I said what that first equation describes. That first equation describes for you a particle in a box. We've forgotten about everything else. So if I have a particle in a box, what is the characteristic time? It has to be set by the size of the box, given that I am moving with that velocity.

So there is a timescale that I would call extrinsic in the sense that it is not really a property of the gas. It will be different if I make the box bigger. There's a timescale over which I would go from one side of the box to another side of the box. So this is kind of a timescale that is related to the term that knows something about the box, which is dU by dq , d by dp . I would say that if I were to assign some typical

magnitude to this type of term, I would say that it is related to having to traverse a distance that is of the order of the size of the box, given the velocity that I have specified. This is an inverse timescale. Right?

And let's sort of imagine that I have an-- and I will call this timescale $1/\tau_U$, because it is sort of determined by my external U . Let's say we have a typical size that is of the order of millimeter. If I make it larger, it will be larger. So actually, let's say we have 10^{-3} meters.

Actually, let's make it bigger. Let's make it of the order of 10^{-1} meter. Kind of reasonable-sized box. Then you would say that this $1/\tau_c$ is of the order of 10^2 divided by 10^{-1} , which is of the order of 1,000. Basically, it takes a millisecond to traverse a box that is a fraction of a meter with these velocities. OK?

You say fine. That is the kind of timescale that I have in the first equation that I have in my hierarchy. And that kind of term is certainly also present in the second equation for the hierarchy. If I have two particles, maybe these two particles are orbiting each other, et cetera. Still, their center of mass would move, typically, with this velocity. And it would take this amount of time to go across the size of the box.

But there is another timescale inside there that I would call intrinsic, which involves dV/dq , d by dp . Now, if I was to see what the characteristic magnitude of this term is, it would have to be V divided by a lens scale that characterizes the potential. And the potential, let's say, is of the order of atomic size or molecular size. Let's call it d .

So this is an atomic size-- or molecular size. More correctly, really, it's the range of the interaction that you have between particles. And typical values of these [? numbers ?] are of the order of 10 angstroms, or angstroms, or whatever. Let's say 10^{-10} meters. Sorry. The first one I would like to call τ_U .

This second time, that I will call $1/\tau_c$ for collisions, is going to be the ratio of 10^2 to 10^{-10} . It's of the order of 10^{12} in both seconds. OK?

So you can see that this term is much, much larger in magnitude than the term that was governing the first equation. OK? And roughly, what you expect in a situation such as this-- let's imagine, rather than shooting particles from here, you are shooting bullets. And then the bullets would come and basically have some kind of trajectory, et cetera.

The characteristic time for a single one of them would be basically something that is related to the size of the box. How long does it take a bullet to go over the size of the box? But if two of these bullets happen to come together and collide, then there's a very short period of time over which they would go in different directions. And the momenta would get displaced from what they were before. And that timescale is of the order of this.

But in the situation that I set up, this particular time is too rapid. There is another more important time, which is, how long do I have to wait for two of these particles, or two of these bullets, to come and hit each other? So it's not the duration of the collision that is irrelevant, but how long it would be for me to find another particle to collide with.

And actually, that is what is governed by the terms that I have on the other side. Because the terms on the other side, what they say is I have to find another particle. So if I look at the terms that I have on the right-hand side and try to construct a characteristic time out of them, I have to compare the probability that I will have, or the density that I will have for $s + 1$, integrated over some volume, over which the force between these particles is non-zero.

And then in order to construct a timescale for it, I know that the d by dt on the left-hand side acts on f_s . On the right-hand side, I have f_{s+1} . So again, just if I want to construct dimensionally, it's a ratio that involves $s + 1$ to s . OK?

So I have to do an additional integration over a volume in phase space over which two particles can have substantial interactions. Because that's where this $[? dv ?]$ by dq would be non-zero, provided that there is a density for $s + 1$ particle compared to s particles. If you think about it, that means that I have to look at the

typical density or particles times d cubed for these additional operations multiplied by this collision time that I had before. OK? And this whole thing I will call 1 over τ collision.

And another way of getting the same result is as follows. This is typically how you get collision times by pictorially. You say that I have something that can interact over some characteristic size d . It moves in space with velocity v so that if I wait a time that I will call τ , within that time, I'm essentially sweeping a volume of space that has volume d squared v τ . So my cross section, if my dimension is d , is d squared. I sweep in the other direction by d τ .

And how many particles will I encounter? Well, if I know the density, which is the number of particles per unit volume, I have to multiply this by n . So how far do I have to go until I hit 1? I'll call that τ_x . Then my formula for τ_x would be 1 over $n d$ squared, which is exactly what I have here. 1 over τ_x is $n d$ squared v . OK?

So in order to compare the terms that I have on the right-hand side with the terms on the left-hand side, I notice that I need to know something about $n d$ cubed. So $n d$ cubed tells you if I have a particle here and this particle has a range of interactions that I call d , how many other particles fall within that range of interaction?

Now, for the gas in this room, the range of the interaction is of the order of the size of the molecule. It is very small. And the distance between molecules in this room is far apart. And indeed, you can estimate that for gas, $n d$ cubed has to be of the order of 10 to the minus 4 .

And how do I know that? Because if I were to take all of the gas particles in this room and put them together so that they are touching, then I would have a liquid. And the density of, say, typical liquid is of the order of $10,000$ times larger than the density of air. So basically, it has to be a number of this order. OK?

So fine. Let's look at our equations. So what I find is that in this equation for f_2 , on the left-hand side, I have a term that has magnitude that is very large-- 1 over τ c . Whereas the term on the right-hand side, in terms of magnitude, is something like

this.

And in fact, this will be true for every equation in the hierarchy. So maybe if I am in the limit where nd^3 is much, much less than 1-- such as the gas in this room, which is called the dilute limit-- I can ignore the right-hand side. I can set the right-hand side to 0. OK?

Now, I can't do that for the first equation, because the first equation is really the only equation in the hierarchy that does not have the collision term on the left-hand side. Right? And so for the first equation, I really need to keep that. And actually, it goes back to all of the story that we've had over here. Remember that we said this ρ equilibrium has to be a function of H and conserved quantities.

Suppose I go to my Hamiltonian and I ignore all of these interactions, which is what I would have done if I just look at the first term over here and set the collision term on the right-hand side to 0. What would happen then? Then clearly, for each one of the particles, I have-- let's say its energy is going to be conserved. Maybe the magnitude of its momentum is going to be conserved in the appropriate geometry. And so there will be a huge number of individual conserved quantities that I would have to put over there.

Indeed, if I sort of go back to the picture that I was drawing over here, if I ignore collisions between the particles, then the bullets that I send will always be following a trajectory such as this forever, because momentum will be conserved. You will always-- I mean, except up to reflection. And say the magnitude of velocity would be always following the same thing. OK?

So however, if there is a collision between two of the particles-- so the particles that come in here, they have different velocities, they will hit each other. The moment they hit each other, they go off different directions. And after a certain number of hits, then I will lose all of the regularity of what I had in the beginning.

And so essentially, this second term on the right-hand with the collisions is the thing that is necessary for me to ensure that my gas does come to equilibrium in the

sense that their momenta get distributed and reversed. I really need to keep track of that. And also, you can see that the timescales for which this kind of equilibration takes place has to do with this collision time.

But as far as this term is concerned, for the gas or for that system of bullets, it doesn't really matter. Because for this term to have been important, it would have been necessary for something interesting to physically occur should three particles come together simultaneously.

And if I complete the-- say that never in the history of this system three particles will come together, they do come together in reality. It's not that big a difference. It's only a factor of 10 to the 4 difference between the right-hand side and the left-hand side. But still, even if they didn't, there was nothing about equilibration of the gas that would be missed by this.

So it's a perfectly reasonable approximation and assumption, therefore, for us to drop this term. And we'll see that although that is physically motivated, it actually doesn't resolve this question of irreversibility yet, because that's also potentially a system that you could set up. You just eliminate all of the three-body interactions from the problem. Still, you could have a very reversible set of conditions and deterministic process that you could reverse in time. But still, it's sort of allows us to have something that is more manageable, which is what we will be looking at next.

Before I go to what is next, I also mentioned that there is one other limit where one can do things, which is when, within the range of interaction of one particle, there are many other particles. So you are in the dense limit, nd^3 greater than 1. This does not happen for a liquid, because for a liquid, the range does not allow many particles to come within it. But it happens for a plasma where you have long-range Coulomb interaction. And within the range of Coulomb interaction, you could have many other interactions.

And so that limit you will explore in the problem set leads to a different description of approach to equilibrium. It's called the Vlasov equation. What we are going to proceed with now will lead to something else, which is called-- in the dilute limit, it

will get the Boltzmann equation. OK?

So let's see what we have. So currently, we achieved something. We want to describe properties of a few particles in the system-- densities that describe only, say, one particle by itself if one was not enough. But I can terminate the equations. And with one-particle density and two-particle density, I should have an appropriate description of how the system evolves.

Let's think about it one more time. So what is happening here? There is the one-particle description that tells you how the density for one particle, or an ensemble, the probability for one particle, its position and momentum evolves. But it requires knowledge of what would happen with a second particle present. But the equations that we have for the density that involves two particles is simply a description of things that you would do if you had deterministic trajectories. There is nothing else on the right-hand side.

So basically, all you need to do is in order to determine this, is to have full knowledge of what happens if two particles come together, collide together, go away, all kinds of things. So if you have those trajectories for two particles, you can, in principle, build this density. It's still not an easy task. But in principle, one could do that. And so this is the description of f_2 . And we expect f_2 to describe processes in which, over a very rapid timescale, say, momenta gets shifted from one direction to another direction. But then there is something about the overall behavior that should follow, more or less, f_1 .

Again, what do I mean? What I mean is the following, that if I open this box, there is what you would observe. The density would kind of gush through here. And so you can have a description for how the density, let's say in coordinate space, would be evolving as a function of time. If I ask how does the two-particle prescription evolve, well, the two-particle prescription, part of it is what's the probability that I have a particle here and a particle there?

And if the two particles, if the separations are far apart, you would be justified to say that that is roughly the product of the probabilities that I have something here and

something there. When you become very close to each other, however, over the range of interactions and collisions, that will have to be modified, because at those descriptions from here, you would have to worry about the collisions, and the exchange of momenta, et cetera.

So in that sense, part of f_2 is simply following f_1 slowly. And part of f_1 captures all of the collisions that you have. In fact, that part of f_2 that captures in the collisions, we would like to simplify as much as possible. And that's the next task that we do.

So what I need to do is to somehow express the f_2 that appears in the first equation while solving this equation that is the second one. I will write the answer that we will eventually deal with and explain it next time. So the ultimate result would be that the left-hand side, we will have the terms that we have currently. f_1 .

On the right-hand side, what we find is that I need to integrate over all momenta of a second particle and something that is like a distance to the target-- one term that is the flux of incoming particles. And then we would have f_2 after collision minus f_2 before collision.

And this is really the Boltzmann equation after one more approximation, where we replace f_2 with f_1 . f_1 . But what all of that means symbolically and what it is we'll have to explain next time.