PROFESSOR: Let's start. Are there any questions? We would like to have a perspective for this really common observation that if you have a gas that is initially in one half of a box, and the other half is empty, and some kind of a partition is removed so that the gas can expand, and it can flow, and eventually we will reach another equilibrium state where the gas occupies more chambers. How do we describe this observation?

We can certainly characterize it thermodynamically from the perspectives of atoms and molecules. We said that if I want to describe the configuration of the gas before it starts, and also throughout the expansion, I would basically have to look at all sets of coordinates and momenta that make up this particle. There would be some point in this [? six ?], and I mention our phase space, that would correspond to where this particle was originally. We can certainly follow the dynamics of this point, but is that useful?

Normally, I could start with billions of different types of boxes, or the same box in a different instance of time, and I would have totally different initial conditions. The initial conditions presumably can be characterized to a density in this phase space. You can look at some volume and see how it changes, and how many points you have there, and define this phase space density row of all of the Q's and P's, and it works as a function of time.

One way of looking at how it works as a function of time is to look at this box and where this box will be in some other instance of time. Essentially then, we are following a kind of evolution that goes along this streamline. Basically, the derivative that we are going to look at involves changes both explicitly in the time variable, and also increasingly to the changes of all of the coordinates and momenta, according to the Hamiltonian that governs the system.

I have to do, essentially, a sum over all coordinates. I would have the change in coordinate i, Qi dot, dot, d row by dQi. Then I would have Pi, dot-- I guess these are all vectors-- d row by dPi. There are six end coordinates that implicitly depend on time. In principle, if I am following along the streamline, I have to look at all of these things.

The characteristic of evolution, according to some Hamiltonian, was that this volume of phase space does not change. Secondly, we could characterize, once we wrote Qi dot, as dH by dP, and the i dot as the H by dQ. This combination of derivatives essentially could be captured, and be written as 0 by dt is the Poisson bracket of H and [? P. ?]

One of the things, however, that we emphasize is that as far as evolution according to a Hamiltonian and this set of dynamics is concerned, the situation is completely reversible in time so that some intermediate process, if I were to reverse all of the momenta, then the gas would basically come back to the initial position. That's true. There is nothing to do about it.

That kind of seems to go against the intuition that we have from thermodynamics. We said, well, in practical situations, I really don't care about all the six end pieces of information that are embedded currently in this full phase space density. If I'm really trying to physically describe this gas expanding, typically the things that I'm interested in are that at some intermediate time, whether the particles have reached this point or that point, and what is this streamline velocity that I'm seeing before the thing relaxes, presumably, eventually into zero velocity?

There's a lot of things that I would need to characterize this relaxation process, but that is still much, much, much less than all of the information that is currently encoded in all of these six end coordinates and momenta. We said that for things that I'm really interested in, what I could, for example, look at, is a density that involves only one particle. What I can do is to then integrate over all of the positions and coordinates of particles that I'm not interested in.

I'm sort of repeating this to introduce some notation so as to not to repeat all of these integration variables, so I will call dVi the phase place contribution of particle i. What I may be interested in is that this is something that, if I integrate over P1 and Q1, it is clearly normalized to unity because my row, by definition, was normalized to unity. Typically we may be interested in something else that I call F1, P1 Q1 P, which is simply n times this-- n times the integral product out i2 to n, dVi, the full row.

Why we do that is because typically you are interested or used to calculating things in [? terms ?] of a number density, like how many particles are within some small volume here, defining the density so that when I integrate over the entire volume of f1, I would get the total number of particles, for example. That's the kind of normalization that people have used for f. More generally, we also introduced fs, which depended on coordinates representing s sets of points, or s particles, if you like, that was normalized to be--

We said, OK, what I'm really interested in, in order to calculate the properties of the gases it expands in terms of things that I'm able to measure, is f1. Let's write down the time evolution of f1. Actually, we said, let's write down the time evolution of fs, along with it. So there's the time evolution of fs. If I were to go along this stream, it would be the fs by dt, and then I would have contributions that would correspond to a the changes in coordinates of these particles.

In order to progress along this direction, we said, let's define the total Hamiltonian. We will have a simple form, and certainly for the gas, it would be a good representation. I have the kinetic energies of all of the particles. I have the box that confines the particles, or some other one particle potential, if you like, but I will write in this much. Then you have the interactions between all pairs of particles. Let's write it as sum over i, less than j, V of Qi minus Qj. This depends on n set of particles, coordinates, and momenta.

Then we said that for purposes of manipulations that you have to deal with, since there are s coordinates that are appearing here whose time derivatives I have to

look at, I'm going to simply rewrite this as the contribution that comes from those s particles, the contribution that comes from the remaining n minus s particles, and some kind of [? term ?] that covers the two sets of particles. This, actually, I didn't quite need here until the next stage because what I write here could, presumably, be sufficiently general, like we have here some n running from 1 to s. Let me be consistent with my S's. Then I have Qn, dot, dFs by dQn, plus Pn, dot, dFs by dPn.

If I just look at the coordinates that appear here, and say, following this as they move in time, there is the explicit time dependence on all of the implicit time dependence, this would be the total derivative moving along the streamline. Qn dot I know is simply the momentum. It is the H by dPn. The H by dPn I have from this formula over here. It is simply Pn divided by m. It's the velocity-- momentum divided by mass. This is the velocity of the particle. Pn dot, the rate of change of momentum is the force that is acting on the particle.

What I need to do is to take the derivatives of various terms here. So I have minus dU by dPn. What is this? This is essentially the force that the particle feels from the external potential. If you are in the box in this room, It is zero until you hit the edge of the box. I will call this Fn to represent external potential that is acting on the system.

What else is there? I have the force that will come from the interaction with all other [? guys. ?] I will write here a sum over m, dV of Qm minus Qn, by dQn-- dU by dQm. I'm sorry.

What is this? This Is basically the sum of the forces that is exerted by the n particle on the m particle. Define it in this fashion.

If this was the entire story, what I would have had here is a group of s particles that are dominated by their own dynamics. If there is no other particle involved, they basically have to satisfy the Liouville equation that I have written, now appropriate to s particles. Of course, we know that that's not the entire story because there are all these other terms involving the interactions with particles that I have not included.

That's the whole essence of the story. Let's say I want to think about one or two particles. There is the interaction between the two particles, and they would be evolving according to some trajectories. But there are all of these other particles in the gas in this room that will collide with them.

So those conditions are not something that we had in the Liouville equation, with everything considered. Here, I have to include the effect of all of those other particles. We saw that the way that it appears is that I have to imagine that there's another particle whose coordinates and momenta are captured through some volume for the s plus 1 particle.

This s plus 1 particle can interact with any of the particles that are in the set that I have on the other side. There is an index that runs from 1 to s. What I would have here is the force that will come from this s plus 1 particle, acting on particle n the same way that this force was deriving the change of the momentum, this force will derive the change of the momentum of-- I guess I put an m here--

The thing that I have to put here is now a density that also keeps track of the probability to find the s plus 1 particle in the location in phase place that I need to integrate with both. I have to integrate over all positions. One particle is moving along a straight line by itself, let's say. Then there are all of the other particles in the system. I have to ask, what is the possibility that there is a second particle with some particular momentum and coordinate that I will be interacting with.

This is the general set up of these D-B-G-K-Y hierarchy of equations. At this stage, we really have just rewritten what we had for the Liouville equation. We said, I'm really, really interested only one particle [? thing, ?] row one and F1. Let's focus on that. Let's write those equations in more detail

In the first equation, I have that the explicit time dependence, plus the time dependence of the position coordinate, plus the time dependence of the momentum coordinate, which is driven by the external force, acting on this one particle density, which is dependent on p1, q1 at time t. On the right hand side of the equation. I need to worry about a second particle with momenta P2 at position Q2 that will,

therefore, be able to exert a force. Once I know the position, I can calculate the force that particle exerts. What was my notation? The order was 2 and 1, dotted by d by dP1. I need now f2, p1, q2 at time t.

We say, well, this is unfortunate. I have to worry about dependence on F2, but maybe I can get away with things by estimating order of magnitudes of the various terms. What is the left hand side set of operations? The left hand side set of operations describes essentially one particle moving by itself.

If that particle has to cross a distance of this order of L, and I tell you that the typical velocity of these particles is off the order of V, then that time scale is going to be of the order of L over V. The operations here will give me a V over L, which is what we call the inverse of Tau u. This is a reasonably long macroscopic time.

OK, that's fine. How big is the right hand side? We said that the right hand side has something to do with collisions.

I have a particle in my system. Let's say that particle has some characteristic dimension that we call d. This particle is moving with velocity V. Alternatively, you can think of this particle as being stationary, and all the other particles are coming at it with some velocity V.

If I say that the density of these particles is n, then the typical time for which, as I shoot these particles, they will hit this target is related to V squared and V, the volume of particles. Over time t, I have to consider this times V tau x. V tau xn V squared should be of the order of one. This gave us a formula for tau x. The inverse of tau x that controls what's happening on this side is n V squared V.

Is the term on the right hand side more important, or the term on the left hand side? The term on the right hand side has to do with the two body term. There's a particle that is moving, and then there's another particle with a slightly different velocity that it is behind it. In the absence of collisions, these particles would just go along a straight line. They would bounce off the walls, but the magnitude of their energy, and hence, velocity, would not change from these elastic collisions.

But if the particles can catch up and interact, which is governed by V2, V on the other side, then what happens is that the particles, when they interact, would collide and go different ways. Quickly, their velocities, and momenta, and everything would get mixed up. How rapidly that happens depends on this collision distance, which is much less than the size of the system, and, therefore, the term that you have on the right hand side in magnitude is much larger than what is happening on the left hand side.

There is no way in order to describe the relaxation of the gas that I can neglect collisions between gas particles. If I neglect collisions between gas particles, there is no reason why the kinetic energies of individual particles should change. They would stay the same forever.

I have to keep this. Let's go and look at the second equation in the hierarchy. What do you have? You have d by dT, P1 over m d by d Q1, P2 over m, P d by d Q2. Then we have F1 d by d Q1, plus F2, d by d Q2 coming from the external potential. Then we have the force that the involves the collision between particles one and two.

When I write down the Hamiltonian for two particles, there is going to be already for two particles and interactions between them. That's where the F1 2 comes from. F1 2 changes d by the momentum of particle one. I should write, it's 2 1 that changes momentum of particle two. But as 2 1 is simply minus F1 2, I can put the two of them together in this fashion. This acting on F2 is then equal to something like integral over V3, F3 1, d by dP1, plus F3 2, d by dP2. [INAUDIBLE] on F3 P1 and Q3 [INAUDIBLE].

Are we going to do this forever? Well, we said, let's take another look at the magnitude of the various terms. This term on the right hand side still involves a collision that involves a third particle. I have to find that third particle, so I need to have, essentially, a third particle within some characteristic volume, so I have something that is of that order.

Whereas on the left hand side now, I have a term that from all perspectives, looks

like the kinds of terms that I had before except that it involves the collision between two particles. What it describes is the duration that collision. We said this is of the order of 1 over tau c, which replaces the n over there with some characteristic dimension. Suddenly, this term is very big. We should be able to use that.

There was a question.

AUDIENCE: On the left hand side of both of your equations, for F1 and F2, shouldn't all the derivatives that are multiplied by your forces be derivatives of the effects of momentum? [INAUDIBLE] the coordinates? [INAUDIBLE] reasons?

PROFESSOR: Let's go back here. I have a function that depends on P, Q, and t. Then there's the explicit time derivative, d by dt. Then there is the Q dot here, which will go by d by dQ. Then there's the P dot term that will go by d by dP. All of things have to be there.

I should have derivatives in respect to momenta, and derivatives with respect to coordinate. Dimensions are, of course, important. Somewhat, what I write for this and for this should make up for that. As I have written it now, it's obvious, of course.

This has dimensions of Q over T. The Q's cancel. I would have one over T. D over Dps cancel. I have 1 over P. Here, dimensionality is correct. I have to just make sure I haven't made a mistake. Q dot is a velocity. Velocity is momentum divided by mass. So that should dimensionally work out. P dot is a force. Everything here is force. In a reasonable coordinate--

AUDIENCE: [INAUDIBLE]

PROFESSOR: What did I do here? I made mistakes?

AUDIENCE: [INAUDIBLE]

PROFESSOR: Why didn't you say that in a way that-- If I don't understand the question, please correct me before I spend another five minutes. Hopefully, this is now free of these deficiencies.

This there is very big. Now, compared to the right hand side in fact, we said that the right hand side is smaller by a factor that measures how many particles are within an interaction volume. And for a typical gas, this would be a number that's of the order of 10 to the minus 4. Using 10 to the minus 4 being this small, we are going to set the right hand side to zero. Now, I don't have to write the equation for F2.

I'll answer a question here that may arise, which is ultimately, we will do sufficient manipulations so that we end up with a particular equation, known as the Boltzmann Equation, that we will show does not obey the time reversibility that we wrote over here. Clearly, that is built in to the various approximations I make.

The first question is, the approximation that I've made here, did I destroy this time reversibility? The answer is no. You can look at this set of equations, and do the manipulations necessary to see what happens if P goes to minus P. You will find that you will be able to reverse your trajectory without any problem. Yes?

AUDIENCE: Given that it is only an interaction from our left side that's very big, that's the reason why we can ignore the stuff on the right. Why is it that we are then keeping all of the other terms that were even smaller before?

PROFESSOR: I will ignore them. Sure.

AUDIENCE: [LAUGHTER]

PROFESSOR: There was the question of time reversibility. This term here has to do with three particles coming together, and how that would modify what we have for just two-body collisions. In principle, there is some probability to have three particles coming together and some combined interactions. You can imagine some fictitious model, which in addition to these two-body interactions, you cook up some body interaction so that it precisely cancels what would have happened when three particles come together.

We can write a computer program in which we have two body conditions. But if three bodies come close enough to each other, they essentially become ghosts and

pass through each other. That computer program would be fully reversible. That's why sort of dropping this there is not causing any problems at this point.

What is it that you have included so far? What we have is a situation where the change in F1 is governed by a process in which I have a particle that I describe on the left hand side with momentum one, and it collides with some particle that I'm integrating over, but in some particular instance of integration, has momentum P2. Presumably they come close enough to each other so that afterwards, the momenta have changed over so that I have some P1 prime, and I have some P2 prime.

We want to make sure that we characterize these correctly. There was a question about while this term is big, these kinds of terms are small. Why should I basically bother to keep them? It is reasonable.

What we are following here are particles in my picture that were ejected by the first box, and they collide into each other, or they were colliding in the first box. As long as you are away from the [? vols ?] of the container, you really don't care about these terms. They don't really moved very rapidly.

This is the process of collision of two particles, and it's also the same process that is described over here. Somehow, I should be able to simplify the collision process that is going on here with the knowledge that the evolution of two particles is now completely deterministic. This equation by itself says, take two particles as if they are the only thing in the universe, and they would follow some completely deterministic trajectory, that if you put lots of them together, is captured through this density.

Let's see whether we can massage this equation to look like this equation. Well, the force term, we have, except that here we have dP by P1 here. We have d by dP 1 minus d by dP2. So let's do this. Minus d by dP2, acting on F2.

Did I do something wrong? The answer is no, because I added the complete derivative over something that I'm integrating over. This is perfectly legitimate mathematics.

This part now looks like this. I have to find what is the most important term that matches this. Again, let's think about this procedure. What I have to make sure of is what is the extent of the collision, and how important is the collision?

If I have one particle moving here, and another particle off there, they will pass each other. Nothing interesting could happen. The important thing is how close they come together. It Is kind of important that I keep track of the relative coordinate, Q, which is Q2 minus Q1, as opposed to the center of mass coordinate, which is just Q1 plus Q2 over 2.

That kind of also indicates maybe it's a good thing for me to look at this entire process in the center of mass frame. So this is the lab frame. If I were to look at this same picture in the center of mass frame, what would I have?

In the center of mass frame, I would have the initial particle coming with P1 prime, P1 minus P center of mass. The other particle that you are interacting with comes with P2 minus P center of mass. I actually drew these vectors that are hopefully equal and opposite, because you know that in the center of mass, one of them, in fact, would be P1 minus P2 over 2. The other would be P2 minus P1 over 2. They would, indeed, in the center of mass be equal and opposite momenta.

Along the direction of these objects, I can look at how close they come together. I can look at some coordinate that I will call A, which measures the separation between them at some instant of time. Then there's another pair of coordinates that I could put into a vector that tells me how head to head they are. If I think about they're being on the center of mass, two things that are approaching each other, they can either approach head on-- that would correspond to be equal to 0-- or they could be slightly off a head-on collision. There is a so-called impact parameter B, which is a measure of this addition fact.

Why is that going to be relevant to us? Again, we said that there are parts of this expression that all of the order of this term, they're kind of not that important. If I think about the collision, and what the collision does, I will have forces that are significant when I am within this range of interactions, D. I really have to look at what

happens when the two things come close to each other.

It Is only when this relative parameter A has approached D that these particles will start to deviate from their straight line trajectory, and presumably go, to say in this case, P2 prime minus P center of mass. This one occurs [? and ?] will go, and eventually P1 prime minus P center of mass. These deviations will occur over a distance that is of the order of this collision and D.

The important changes that occur in various densities, in various potentials, et cetera, are all taking place when this relative coordinate is small. Things become big when the relative coordinate is small. They are big as a function of the relative coordinate.

In order to get big things, what I need to do is to replace these d by dQ's with the corresponding derivatives with respect to the center of mass. One of them would come be the minus sign. The other would come be the plus sign. It doesn't matter which is which. It depends on the definition, whether I make Q2 minus Q1, or Q1 minus Q2.

We see that the big terms are the force that changes the momenta and the variations that you have over these relative coordinates. What I can do now is to replace this by equating the two big terms that I have over here. The two big terms are P2 minus P1 over m, dotted by d by dQ of F2.

There is some other approximation that I did. As was told to me before, this is the biggest term, and there is the part of this that is big and compensates for that. But there are all these other bunches of terms. There's also this d by dt.

What I have done over here is to look at this slightly coarser perspective on time. Increasing all the equations that I have over there tells me everything about particles approaching each other and going away. I can follow through the mechanics precisely everything that is happening, even in the vicinity of this collision.

If I have two squishy balls, and I run my hand through them properly, I can see how

the things get squished then released. There's a lot of information, but again, a lot of information that I don't really care to know as far as the properties of this gas expansion process is concerned. What you have done is to forget about the detailed variations in time and space that are taking place here. We're going to shortly make that even more explicit by noting the following.

This integration over here is an integration over phase space of the second particle. I had written before d cubed, P2, d cubed, Q2, but I can change coordinates and look at the relative coordinate, Q, over here. What I'm asking is, I have one particle moving through the gas. What is the chance that the second particle comes with momentum P2, and the appropriate relative distance Q, and I integrate over both the P and the relative distance Q? This is the quantity that I have to integrate.

Let's do one more calculation, and then we will try to give a physical perspective. In this picture of the center of mass, what did I do? I do replaced the coordinate, Q, with a part that was the impact parameter, which had two components, and a part that was the relative distance.

What was this relative distance? The relative distance was measured along this line that was giving me the closest approach. What is the direction of this line? The direction of this line is P1 minus P2. This is P1 minus P2 over 2. It doesn't matter. The direction is P1 minus P2.

What I'm doing here is I am taking the derivative precisely along this line of constant approach. I'm taking a derivative, and I'm integrating along that. If I were to rewrite the whole thing, what do I have? I have d by dt, plus P1 over m, d by dQ1, plus F1, d by dP1-- don't make a mistake-- acting on F1, P1, Q1, t.

What do I have to write on the right hand side? I have an integral over the momentum of this particle with which I'm going to make a collision. I have an integral over the impact parameter that tells me the distance of closest approach. I have to do the magnitude of P2 minus P1 over n, which is really the magnitude of the relative velocity of the two particles. I can write it as P2 minus P1, or P1 minus P2.

These are, of course, vectors. and I look at the modulus. I have the integral of the derivative. Very simply, I will write the answer as F2 that is evaluated at some large distance, plus infinity minus F2 evaluated at minus infinity. I have infinity.

In principle, I have to integrate over F2 from minus infinity to plus infinity. But once I am beyond the range of where the interaction changes, then the two particles just move away forever. They will never see each other.

Really, what I should write here is F2 of-- after the collision, I have P1 prime, P2 prime, at some Q plus, minus F2, P1, P2, at some position minus. What I need to do is to do the integration when I'm far away from the collision, or wait until I am far after the collision. Really, I have to just integrate slightly below, after, and before the collision occurs. In principle, if I just go a few d's in one direction or the other direction, this should be enough.

Let's see physically what this describes. There is a connection between this and this thing that I had over here, in fact. This equation on the left hand side, if it was zero, it would describe one particle that is just moving by itself until it hits the wall, at which point it basically reverses its trajectory, and otherwise goes forward.

But what you have on the right hand side says that suddenly there could be another particle with which I interact. Then I change my direction. I need to know the probability, given that I'm moving with velocity P1, that there is a second particle with P2 that comes close enough.

There is this additional factor. From what does this additional factor come? It's the same factor that we have over here. It is, if you have a target of size d squared, and we have a set of bullets with a density of n, the number of collisions that I get depends both on density and how fast these things go. The time between collisions, if you like, is proportional to n, and it is also related to V. That's what this is.

I need some kind of a time between the collisions that I make. I have already specified that I'm only interested in the set of particles that have momentum P2 for

this particular [? point in ?] integration, and that they have this kind of area or cross section. So I replace this V squared and V with the relative coordinates.

This is the corresponding thing to V squared, and this is really a two particle density. This is a subtraction. The addition is because it is true that I'm going with velocity P1, and practically, any collisions that are significant will move me off kilter. So there has to be a subtraction for the channel that was described by P1 because of this collision.

This then, is the addition, because it says that it could be that there is no particle going in the horizontal direction. I was actually coming along the vertical direction. Because of the collision, I suddenly was shifted to move along this direction. The addition comes from having particles that would correspond to momenta that somehow, if I were in some sense to reverse this, and then put a minus sign, a reverse collision would create something that was along the direction of P1.

Here I also made several approximations. I said, what is chief among them is that basically I ignored the details of the process that is taking place at scale the order of d, so I have thrown away some amount of detail and information. It is, again, legitimate to say, is this the stage at which you made an approximation so that the time reversibility was lost? The answer is still no. If you are careful enough with making precise definitions of what these Q's are before and after the collision, and follow what happens if you were to reverse everything, you'll find that the equations is fully reversible.

Even at this stage, I have not made any transition. I have made approximations, but I haven't made something to be time irreversible. That comes at the next stage where we make the so-called assumption of molecular chaos.

The assumption is that what's the chance that I have a particle here and a particle there? You would say, it's a chance that I have one here and one there. You say that if two of any P1, P2, Q1, Q2, t is the same thing as the product of F1, P1, Q1, t, F1, P2, Q2, t.

Of course, this assumption is generally varied. If I were to look at the probability that I have two particles as a function of, let's say, the relative separation, I certainly expect that if they are far away, the density should be the product of the one particle densities. But you would say that if the two particles come to distances that are closer than their separation d, then the probability and the range of interaction d-- and let's say the interaction is highly repulsive like hardcore-- then the probability should go to 0. Clearly, you can make this assumption, but up to some degree.

Part of the reason we went through this process was to indeed make sure that we are integrating things at the locations where the particles are far away from each other. I said that the range of that integration over A would be someplace where they are far apart after the collision, and far apart before the collision. You have an assumption like that, which is, in principle, something that I can insert into that.

Having to make a distinction between the arguments that are appearing in this equation is kind of not so pleasant. What you are going to do is to make another assumption. Make sure that everything is evaluated at the same point.

What we will eventually now have is the equation that d by dt, plus P1 over n, d by dQ1, plus F1, dot, d by dP1, acting on F1, on the left hand side, is, on the right hand side, equal to all collisions in the particle of momentum P2, approaching at all possible cross sections, calculating the flux of the incoming particle that corresponds to that channel, which is proportional to V2 minus V1. Then here, we subtract the collision of the two particles. We write that as F1 of P1 at this location, Q1, t, F1 of t2 at the same location Q1, t. Then add F1 prime, P1 prime, Q1 t, F1 prime, P2 prime, Q2, t.

In order to make the equation eventually manageable, what you did is to evaluate all off the coordinates that we have on the right hand side at the same location, which is the same Q1 that you specify on the left hand side. That immediately means that what you have done is you have changed the resolution with which you are looking at space. You have kind of washed out the difference between here and here. Your resolution has to put this whole area that is of the order of d squared or

d cubed in three dimensions into one pixel. You have changed the resolution that you have. You are not looking at things at this [? fine ?] [? state. ?]

You are losing additional information here through this change of the resolution in space. You have also lost some information in making the assumption that the two [? point ?] densities are completely within always as the product one particle densities. Both of those things correspond to taking something that is very precise and deterministic, and making it kind of vague and a little undefined.

It's not surprising then, that if you have in some sense changed the precision of your computer-- let's say, that is running the particles forward-- at some point, you've changed the resolution. Then you can't really run backward. In fact, to sort of precisely be able to run the equations forward and backward, you would need to keep resolution at all levels. Here, we have sort of removed some amount of resolution. We have a very good guess that the equation that you have over here no longer respects time reversal inversions that you had originally posed.

Our next task is to prove that you need this equation. It goes in one particular direction in time, and cannot be drawn backward, as opposed to all of the predecessors that I had written up to this point. Are there any questions?

AUDIENCE: [INAUDIBLE]

PROFESSOR: Yes, Q prime and Q1, not Q1 prime. There is no dash.

AUDIENCE: Oh, I see. It is Q1.

PROFESSOR: Yes, it is. Look at this equation. On the left hand side, what are the arguments? The arguments are P1 and Q1. What is it that I have on the other side? I still have P1 and Q1. I have introduced P1 and b, which is simply an impact parameter. What I will do is I will evaluate all of these things, always at the same location, Q1. Then I have P1 and P2. That's part of my story of the change in resolution. When I write here Q1, and you say Q1 prime, but what is Q1 prime? Is it Q1 plus b? Is it Q1 minus b? Something like this I'm going to ignore.

It's also legitimate, and you should ask, what is P1 prime and Q2 prime? What are they? What I have to do, is I have to run on the computer or otherwise, the equations for what happens if I have P1 and P2 come together at an impact parameter that is set by me. I then integrate the equations, and I find that deterministically, that collision will lead to some P1 prime and P2 prime.

P1 prime and P2 prime are some complicated functions of P1, P2, and b. Given that you know two particles are approaching each other at distance d with momenta P1 P2, in principle, you can integrate Newton's equations, and figure out with what momenta they end up. This equation, in fact, hides a very, very complicated function here, which describes P1 prime and P2 prime as a function of P1 and P2.

If you really needed all of the details of that function, you would surely be in trouble. Fortunately, we don't. As we shall see shortly, you can kind of get a lot of mileage without knowing that. Yes, what is your question?

AUDIENCE: There was an assumption that all the interactions between different molecules are central potentials [INAUDIBLE]. Does the force of the direction between two particles lie along the [INAUDIBLE]?

PROFESSOR: For the things that I have written, yes it does. I should have been more precise. I should have put absolute value here.

AUDIENCE: You have particles moving along one line towards each other, and b is some arbitrary vector. You have two directions, so you define a plane. Opposite direction particles stay at the same plane. Have you reduced--

PROFESSOR: Particles stay in the same plane?

AUDIENCE: If the two particles were moving towards each other, and also you have in the integral your input parameter, which one is [INAUDIBLE]. There's two directions. All particles align, and all b's align. They form a plane. [? Opposite ?] direction particles [? stand ?] in the--

PROFESSOR: Yes, they stand in the same plane.

AUDIENCE: My question is, what is [INAUDIBLE] use the integral on the right from a two-dimensional integral [? in v ?] into employing central symmetry?

PROFESSOR: Yes, you could. You could, in principle, write this as b db, if you like, if that's what you want.

AUDIENCE: [INAUDIBLE]

PROFESSOR: Yes, you could do that if you have simple enough potential.

Let's show that this equation leads to irreversibility. That you are going to do here. This, by the way, is called the Boltzmann equation.

There's an associated Boltzmann H-Theorem, which restates the following-- If F of P1, Q1, and t satisfies the above Boltzmann equation, then there is a quantity H that always decreases in time, where H is the integral over P and Q of F1, log of F1. The composition of irreversibility, as we saw in thermal dynamics, was that there was a quantity entropy that was always increasing. If you have calculated for this system, entropy before for the half box, and entropy afterwards for the space both boxes occupy, the second one would certainly be larger.

This H is a quantity like that, except that when it is defined this way, it always decreases as a function of time. But it certainly is very much related to entropy. You may have asked, why did Boltzmann come across such a function, which is F log F, except that actually right now, you should know why you write this.

When we were dealing with probabilities, we introduced the entropy of the probability distribution, which was related to something like sum over iPi, log of Pi, with a minus sign. Up to this factor of normalization N, this F1 really is a one-particle probability. After this normalization N, you have a one-particle probability, the probability that you have occupation of one-particle free space. This occupation of one-particle phase space is changing as a function of time. What this statement says is that if the one-particle density evolves in time according to this equation, the corresponding minus entropy decreases as a function of time.

Let's see if that's the case. To prove that, let's do this. We have the formula for H, so let's calculate the H by dt.

I have an integral over the phase space of particle one, the particle that I just called one. I could have labeled it anything. After integration, H is only a function of time.

I have to take the time derivative. The time derivative can act on F1. Then I will get the F1 by dt, times log F1. Or I will have F1 times the derivative of log F1. The derivative of log F1 would be dF1 by dt, and then 1 over F1. Then I multiply by F1. This term is simply 1.

AUDIENCE: Don't you want to write the full derivative, F1 with respect [INAUDIBLE]?

PROFESSOR: I thought we did that with this before. If you have something that I am summing over lots of [? points, ?] and these [? points ?] can be positioned, then I have S at location one, S at location two, S at location three, discretized versions of x. If I take the time derivative, I take the time derivative of this, plus this, plus this, which are partial derivatives.

If I actually take the time derivative here, I get the integral d cubed P1, d cubed Q1, the time derivative. This would be that partial dF1 by dt is the time derivative of n, which is 0. The number of particles does not change. Indeed, I realize that 1 integrated against dF1 by dt is the same thing that's here. This term gives you 0.

All I need to worry about is integrating log F against the Fydt. I have an integral over P1 and Q1 of log F against the Fydt. We have said that F1 satisfies the Boltzmann equation.

So the F1 by dt, if I were to rearrange it, I have the F1 by dt. I take this part to the other side of the equation. This part is also the Poisson bracket of a one-particle H with F1. If I take it to the other side, it will be the Poisson bracket of H with F1.

Then there is this whole thing that involves the collision of two particles. So I define whatever is on the right hand side to be some collision operator that acts on two [? powers ?] of F1. This is plus a collision operator, F1, F1. What I do is I replace this

dF1 by dt with the Poisson bracket of H, or H1, if you like, with F1. The collision operator I will shortly write explicitly. But for the time being, let me just write it as C of F1.

There is a first term in this sum-- let's call it number one-- which I claim to be 0. Typically, when you get these integrations with Poisson brackets, you would get 0. Let's explicitly show that. I have an integral over P1 and Q1 of log of F1, and this Poisson bracket of H1 and F1, which is essentially these terms. Alternatively, I could write it as dH1 by dQ1, dF1 by dt1, minus the H1 by dt1, dF1, by dQ1.

I've explicitly written this form for the one-particle in terms of the Hamiltonian. The advantage of that is that now I can start doing integrations by parts. I'm taking derivatives with respect to P, but I have integrations with respect to P here.

I could take the F1 out. I will have a minus. I have an integral, P1, Q1. I took F1 out. Then this d by dP1 acts on everything that came before it.

It can act on the H1. I would get d2 H1 with respect to dP1, dQ1. Or it could act on the log of F1, in which case I will get set dH1 by dQ1. Then I would have d by dP acting on log of F, which would give me dF1 by dP1, then the derivative of the log, which is 1 over F1.

This is only the first term. I also have this term, with which I will do the same thing.

AUDIENCE: [INAUDIBLE] The second derivative [INAUDIBLE] should be multiplied by log of F.

PROFESSOR: Yes, it should be. It is Log F1. Thank you.

For the next term, I have F1. I have d2 H1, and the other order of derivatives, dQ1, dP1. Now I'll make sure I write down the log of F1. Then I have dH1 with respect to dQ1. Then I have a dot product with the derivative of log F, which is the derivative of F1 with respect to Q1 and 1 over F1.

Here are the terms that are proportional to the second derivative. The order of the derivatives does not matter. One often is positive. One often is negative, so they cancel out.

Then I have these additional terms. For the additional terms, you'll note that the F1 and the 1 over F1 cancels. These are just a product of two first derivatives.

I will apply the five parts process one more time to get rid of the derivative that is acting on F1. The answer becomes plus d cubed P1, d cubed Q1. Then I have F1, d2 H1, dP1, dQ1, minus d2 H1, dQ1, dP1. These two cancel each other out, and the answer is 0.

So that first term vanishes. Now for the second term, number two, what I have is the first term vanished. So I have the H by dt. It is the integral over P1 and Q1. I have log of F1. F1 is a function of P1, and Q1, and t. I will focus, and make sure I write the argument of momentum, for reasons that will become shortly apparent.

I have to multiply with the collision term. The collision term involves integrations over a second particle, over an impact parameter, a relative velocity, once I have defined what P2 and P1 are. I have a subtraction of F evaluated at P1, F evaluated at P2, plus addition, F evaluated at P1 prime, F evaluated at P2 prime.

Eventually, this whole thing is only a function of time. There are a whole bunch of arguments appearing here, but all of those arguments are being integrated over. In particular, I have arguments that are indexed by P1 and P2. These are dummy variables of integration. If I have a function of x and y that I'm integrating over x and y, I can call x "z." I can call y "t." I would integrate over z and t, and I would have the same answer.

I would have exactly the same answer if I were to call all of the dummy integration variable that is indexed 1, "2." Any dummy variable that is indexed 2, if I rename it and call it 1, the integral would not change. If I do that, what do I have? I have integral over Q-- actually, let's get of the integration number on Q. It really doesn't matter.

I have the integrals over P1 and P1. I have to integrate over both sets of momenta. I have to integrate over the cross section, which is relative between 1 and 2. I have

V2 minus V1, rather than V1 minus V2, rather than V2 minus V1. The absolute value doesn't matter. If I were to replace these indices with an absolute value, [? or do a ?] V2 minus V1 goes to minus V1 minus V2. The absolute value does not change.

Here, what do I have? I have minus F of P1. It becomes F of P2, F of P1, plus F of P2 prime, f of P1 prime. They are a product. It doesn't really matter in which order I write them. The only thing that really matters is that the argument was previously called F1 of P1 for the log, and now it will be called F1 of P2. Just its name changed.

If I take this, and the first way of writing things, which are really two ways of writing the same integral, and just average them, I will get 1/2 an integral d cubed Q, d cubed P1, d cubed P2, d2 b, and V2 minus V1. I will have F1 of P1, F1 of P2, plus F1 of P1 prime, F1 of P2 prime. Then in one term, I had log of F1 of P1, and I averaged it with the other way of writing things, which was log of F-- let's put the two logs together, multiplied by F1. So the sum of the two logs I wrote, that's a log of the product. I just rewrote that equation. If you like, I symmetrized It with respect to index 1 and 2. So the log of 1, that previously had one argument through this symmetrization, became one half of the sum of it.

The next thing one has to think about, what I want to do, is to replace primed and unprimed coordinates. What I would eventually write down is d cubed P1 prime, d cubed P2 prime, d2 b, V2 prime minus V1 prime, minus F1 of P1 prime, F1 of P2 prime, plus F1 of P1, F1 of P2. Then log of F1 of P1 prime, F1 of P2 prime.

I've symmetrized originally the indices 1 and 2 that were not quite symmetric, and I end up with an expression that has variables P1, P2, and functions P1 prime and P2 prime, which are not quite symmetric again, because I have F's evaluated for P's, but not for P primes. What does this mean? This mathematical expression that I have written down here actually is not correct, because what this amounts to, is to change variables of integration.

In the expression that I have up here, P1 and P2 are variables of integration. P1

prime and P2 prime are some complicated functions of P1 and P2. P1 prime is some complicated function that I don't know. P1, P2, and V, for which I need to solve in principle, is Newton's equation. This is similarly for P2 prime.

What I have done is I have changed from my original variables to these functions. When I write things over here, now P1 prime and P2 prime are the integration variables. P1 and P2 are supposed to be regarded as functions of P1 prime and P2 prime.

You say, well, what does that mean? You can't simply take an integral dx, let's say F of some function of x, and replace this function. You can't call it a new variable, and do integral dx prime. You have to multiply with the Jacobian of the transformation that takes you from the P variables to the new variables.

My claim is that this Jacobian of the integration is, in fact, the unit. The reason is as follows. These equations that have to be integrated to give me the correlation are time reversible.

If I give you two momenta, and I know what the outcomes are, I can write the equations backward, and I will have the opposite momenta go back to minus the original momenta. Up to a factor of minus, you can see that this equation has this character, that P1, P2 go to P1 prime, P2 prime, then minus P1 prime, minus P2 prime, go to P1, and P2. If you sort of follow that, and say that you do the transformation twice, you have to get back up to where a sign actually disappears to where you want. You have to multiply by two Jacobians, and you get the same unit. You can convince yourself that this Jacobian has to be unit.

Next time, I guess we'll take it from there. I will explain this stuff a little bit more, and show that this implies what we had said about the Boltzmann equation.