THIRD LECTURE

To remind you where we were, I tried to discuss this problem from what one might say is a purely probabilistic point of view. For I simply said to myself that my system can be in any state described by a vector $\vec{\eta}$ whose components are either plus ones or minus ones. And in each elementary step I can perform a transition from a state $\vec{\delta}$ to a state $\vec{\eta}$, and I would like to calculate the probability of such a transition. In fact, I have already calculated it. Now I might as well write out the equation completely and simply hope for the best:

$$\rho(\vec{\eta}, t+1) = \sum_{\vec{\delta}} \rho(\vec{\delta}, t)\, P(\vec{\delta}|\vec{\eta}) \tag{48}$$

This, as a matter of fact, is exactly the matrix equation (46) written out in its full glory. In this connection it is called the Master equation. In the mathematical literature it is referred to as the Chapman-Kolmogoroff equation. But of course it's just the perfectly obvious consequence of our assumptions.

I am first going to provide myself with a convenient basis in my phase space. Remember that my phase space is a very simple set whose elements are vectors with components that are plus one or minus one. Consider the following functions:

$$1;\ \eta_k;\ \eta_k\eta_l;\ \eta_k\eta_l\eta_m;\ \ldots;\ \eta_1\eta_2\cdots\eta_n \qquad k \leqslant l \leqslant m \leqslant \cdots$$

How many such quantities do I have? It's perfectly obvious that I have n single η's. I have $\binom{n}{2}$ $\eta_k\eta_l$, $k \leqslant l$ etc. So there are exactly

$$1 + n + \binom{n}{2} + \binom{n}{3} + \cdots + \binom{n}{n} = 2^n$$

of these things. I claim that they form a complete set. First of all, what does η_1 mean? η_1 ought to be looked at as a function defined on my space

of all possible sequences of ones and minus ones. It means to always take the first component. That's the function. And $\eta_k \eta_\ell$ always means to take the product of the k th component and the ℓ th component. So we have here 2^n functions defined on the set of all possible sequences of plus ones and minus ones of length n.

Now I claim that every function of the vector $\vec{\eta}$ -- and in particular $\rho(\vec{\eta},0)$ -- can be written in terms of these functions. In fact,

$$\rho(\vec{\eta},0) = \frac{1}{2^n} + \sum C_k \eta_k + \sum C_{k\ell} \eta_k \eta_\ell + \cdots + C_{12\ldots n} \eta_1 \eta_2 \cdots \eta_n \quad (49)$$

This is similar to expanding a function into a series of harmonics. In fact, you can easily find the coefficients by Fourier's formula, if you wish. For instance,

$$C_{k\ell} = \frac{1}{2^n} \sum_{\vec{\eta}} \rho(\vec{\eta}) \eta_k \eta_\ell \quad (50)$$

This formula, and in fact the validity of the expansion, follows from the fact that my functions are orthogonal. The reason I have $\frac{1}{2^n}$ in formula (49) simply goes back to the condition that the sum of all the ρ values must be one. Except for this constant all the terms sum to zero. So the constant must be such that when it is multiplied by 2^n it will give you one; and then, of course, it's $1/2^n$.

And now the question is, what happens if I operate with the matrix on each individual term of the expansion? Let's take a typical term, a very simple one -- let's take $\eta_1 \eta_2$. It's a vector of 2^n components. Now let's apply the matrix P to it and see what happens. The result is

$$P\{\eta_1 \eta_2\} = \sum_{\delta} \delta_1 \delta_2 \prod_{k=1}^{n} \left[\frac{1}{2} + \frac{1-2\mu}{2} \delta_k \eta_{k+1} \right] \quad (51)$$

where we have made use of equation (43'). What does it mean to sum over $\sum_{\delta}$? It means summing over all δ_1 , δ_2 , . . ., δ_n . But now look. What you are summing is a product of independent functions. Hence, in summing, you can simply sum things separately and then multiply to get the answer. It's again like integrating a function of n variables which happens to be a product of functions of individual variables. You know very well that such a thing is just a product of integrals. Now the summation over δ_1 and δ_2 is evidently special. But what is the summation of one of the other factors? When δ_k is + 1 you get

$$\frac{1}{2} + \frac{1-2\mu}{2}\eta_{k+1}$$

and when δ_k is - 1 you get

$$\frac{1}{2} - \frac{1-2\mu}{2}\eta_{k+1}$$

So, if you add them together, you get one. What, however, about the factor that has the δ_1 ? There are only two values for δ_1 , plus one and minus one, so it's going to be

$$(1-2\mu)\eta_2$$

So finally when you perform the whole sum, believe it or not, you're going to get

$$P\{\eta_1\eta_2\} = (1-2\mu)^2\eta_2\eta_3 \qquad (52)$$

Now all this is actually something which one ought to go through by oneself. It's extremely simple, and in fact the symbolism makes it look much deeper than it really is. Yet, if you did not have the symbolism, it would take me three blackboards to write it all out. It is something you can, with the greatest of ease, check for yourself. When the operator P is applied to any of

the terms in the expansion (49) the following two things happen: It multiplies them by $(1-2\mu)$, that means it decreases their length in that proportion. And then it shifts the indices by one. This is in fact a description of the operator P. You saw this happen in the example we went through, and it is easy to show that it is generally so. Now it is very interesting to see what happens if you apply the operator twice. It means multiplying by $(1-2\mu)^4$ and shifting the indices by two. If I apply it t times, then I am simply going to have $(1-2\mu)^{2t}$ and the indices will be shifted by t. There is the usual understanding, that we mentioned before, that if by any chance some number becomes bigger than n, then you simply reduce it modulo n to get back within the range. Now we can immediately write the solution of the Master equation. Everything was constructed so that no trouble could possibly arise and the solution is

$$\rho(\vec{\eta},t)=\frac{1}{2^n}+(1-2\mu)^t\sum_k C_k\eta_{k+t}+(1-2\mu)^{2t}\sum_{k<l}C_{kl}\eta_{k+t}\eta_{l+t}+\cdots$$

$$\cdots+(1-2\mu)^{nt}C_{1,\ldots,n}\eta_{1+t}\eta_{2+t}\cdots\eta_{n+t} \qquad (53)$$

(refer to equation 49).

Now let's take a look at it. This is a very interesting result, because it agrees completely with our intuition. Notice that all the terms except the first one have an exponential tacked to them. So all of them vanish exponentially, as t goes to infinity. And in the limit, you get the distribution $\frac{1}{2^n}$ which is the uniform distribution. This is actually a general feature of all such equations where the matrix P is a stochastic matrix (there are exceptions, but they are minor exceptions) -- If a matrix has all its elements non-negative, and if the sum of the elements in each row is one, such a matrix is called a stochastic matrix. Barring certain exceptions which I am not going to

go into, a high power of such an operator destroys everything except one fundamental eigenvector. All other eigenvectors are annihilated as you easily can see from (53). You have here a very good example of the disappearance of information. My initial distribution $\rho(\vec{\eta},0)$ could have been concentrated on one point -- I could have said it was exactly equal to one at one specific vector, and zero otherwise. So I would know precisely the state of the system at time zero. But at the end, all the states become equally probable. Then I know as little as possible about the system. I started from complete knowledge and ended up with complete ignorance. (This is not unlike the behavior of students, except that their initial state is somewhat different.)

However, all this was based on definitely treating the whole thing by probability methods. Because I simply assumed that I could replace my model by a stochastic model. I said to myself, I don't care what the detailed mechanism is. I will replace my model by a model in which I have at each time interval a transition from a state $\vec{\delta}$ to a state $\vec{\eta}$, with the probability given by a complicated formula. And the only place I used the dynamics of the model was to guess, or to derive if you wish, the formula for the transition probability. I emphasize this, because I am going to follow the same procedure in deriving the Boltzmann equation. I am going to do exactly the same thing.

On this model we can go farther, however. Because we can ask ourselves, can we really justify this probability approach? To answer this question, I must go back to the fundamental problem, whether $\langle L^t \rangle$ is the same as $\langle L \rangle^t$. In general, this is an extremely complicated question. There is now some hope, because there are some partial results. Both in this country and in Russia there are many people who have tried to approach this particular

problem for actual dynamical systems. But the difficulty is that you can never solve the analog of equation (41) -- that is, the Liouville equation which gives you the evolution of the distribution in phase space. It involves all the complications of the equations of motion of a complicated dynamical system. Since it is impossible to solve it rigorously, it seems very difficult at first to see how one could possibly justify the Boltzmann procedure. Here, however, everything is extremely easy. Because the Liouville equation can be solved exactly and I can perform the averaging at the end.

And now let us see what happens. I will still start with exactly the same initial distribution, but now I will use equation (41) and write out the exact formula for $\rho(\vec{\eta},t)$. Here you will discover

$$\rho(\vec{\eta},t) = \frac{1}{2^n} + \sum_p C_p \eta_{p+t} \varepsilon_p \varepsilon_{p+1} \cdots \varepsilon_{p+t-1} + \sum_{p<q} C_{pq} \eta_{p+t} \eta_{q+t} (\varepsilon_p \cdots \varepsilon_{p+t-1})(\varepsilon_q \cdots \varepsilon_{q+t-1}) + \cdots \tag{54}$$

Now of course, the coefficients which are attached to these terms do not decrease exponentially. They are either plus one or minus one, because remember that each ε_p is either plus one or minus one. But that's not surprising after all, because I have not yet performed the average over the positions of the set S. What I have written so far simply represents L^t, the operator raised to the power t. So I must now perform the average over the positions of the set S:

$$\langle \rho(\vec{\eta},t) \rangle = \frac{1}{2^n} + \sum_p C_p \eta_{p+t} \langle \varepsilon_p \varepsilon_{p+1} \cdots \varepsilon_{p+t-1} \rangle + \sum_{p<q} C_{pq} \eta_{p+t} \eta_{q+t} \langle (\varepsilon_p \cdots \varepsilon_{p+t-1})(\varepsilon_q \cdots \varepsilon_{q+t-1}) \rangle + \cdots \tag{55}$$

And now you discover a very interesting thing -- that the first two terms are just the same as before. Because $\langle \varepsilon_p \cdots \varepsilon_{p+t-1} \rangle$ is just an average of a

product. Since I have assumed that the ε_p were chosen independently (remember I flipped a coin to determine at each point p). Consequently,

$$\langle \varepsilon_p \cdots \varepsilon_{p+t-1} \rangle = \langle \varepsilon_p \rangle \cdots \langle \varepsilon_{p+t-1} \rangle = (1-2\mu)^t \tag{56}$$

So the first two terms are exactly what I had before. The trouble begins with the next term. In the next term, notice that you have $(\varepsilon_p \cdots \varepsilon_{p+t-1})$ and $(\varepsilon_q \cdots \varepsilon_{q+t-1})$. If these two groups were entirely separate, if they did not have any ε in common, we could again say that the average of the product is the product of the averages and you would get what you should: $(1-2\mu)^{2t}$. Unfortunately, however, these groups will not be non-overlapping for all of the terms. Let me define

$$\Delta(p,q,t) = \begin{cases} 2t \text{ if } q-p > t \\ 2(p-q) \text{ if } q-p \leq t \end{cases} \tag{57}$$

Now if you calculate this average, you get the following:

$$\langle (\varepsilon_p \cdots \varepsilon_{p+t-1})(\varepsilon_q \cdots \varepsilon_{q+t-1}) \rangle = (1-2\mu)^{\Delta(p,q,t)} \tag{58}$$

What this means is that if p and q are close together the decay factor is $(1-2\mu)^{2(p-q)}$ which does not decay. It stays the same as p goes to infinity. To add insult to injury, the very last term, $\zeta_{12\cdots n}\eta_1 \cdots \eta_n$ won't decay at all. Nothing will happen to it.

Now what is the trouble, and how do we deal with it? One should try to solve Liouville's equation, and one should average. This is definitely correct it is certainly the way one should do the problem. But, lo and behold, you do not get the same result as with the more convenient Boltzmann approach. So this is the real difficulty -- and it occurs also in the actual physical case: What you really want is to use the Boltzmann approach which you know how to handle and apply. But all you really have is Liouville's equation with the

possibility of some averaging. And here you are certainly not led to quite the same result. Fortunately, it is not very serious in this case.

You can talk your way out of it as follows (there are several ways of talking oneself out of it, but we will only look at one of them). Suppose that we start from a symmetric distribution; this means that the function $\rho(\vec{\eta}, 0)$ is a symmetric function in the arguments $\eta_1, \cdots, \eta_n$. In other words, there is no distinction between the points. You don't know which is which. If $\rho(\vec{\eta}, 0)$ is to be a symmetric distribution, then all the C_k's are the same, all the C_{kl}'s are the same, etc. Now even if you start with a symmetric distribution, as you should, then as the thing evolves even that is destroyed. This is because some of the coefficients will be multiplied by $(1-2\mu)^{2t}$ and some will be multiplied by $(1-2\mu)^{p-q}$. Hence, you might say that, in time, the original indistinguishability of sites gets destroyed. In the language of gases, if you wish: At time zero you may not be able to tell which particle is which but by the time they collide a few times it is possible to re-establish their identity. That's not a very pleasant perspective. Consequently, what I should really do is not only to follow the motion in time and then perform an average over the positions of the set S. But in addition to that, I should perform a symmetrization on all the variables η_k.

This is not a logical proof which is independent of how persuasive I am. What I'm saying right now is really a matter of belief, because I have no logical compulsion for it. But you can see that since it is really impossible to follow each particle separately, and know where it is all the time, and what it's color is, that this indistinguishability should be maintained all the time. So now if you also symmetrize -- that is, if you average over all possible

arrangements of the $\eta_1, \ldots, \eta_n$ -- then you will discover the following interesting things. First of all, the two terms we like are not affected. They are just

$$\frac{1}{2^n} + (1-2\mu)^t C_1 \sum_p \eta_p \tag{59}$$

(since all the C_k's are the same, I can take $C_1 = C_k$ outside the sum). Now I want to show you what happens to the terms with which we had difficulty. They become

$$\frac{C_{12} \sum_{1 \leq p \leq q \leq t} (1-2\mu)^{\Delta(p,q,t)}}{\binom{n}{2}} \sum_{1 \leq p \leq q \leq t} \eta_{p+t} \eta_{q+t} \tag{60}$$

Now we like the terms for which $\Delta(p,q,t)$ is equal to $2t$. The terms which we don't like are the ones for which $\Delta(p,q,t)$ is less than $2t$. The number of such terms is only of order n. But the denominator is of order n^2. Consequently, the proportion of objectionable terms is very small -- (remember that n has to go to infinity).

Now the same thing happens for every term. In the next one, we're going to have $\binom{n}{3}$ in the denominator, while the number of undesirables is only going to be of order n^2. Consequently you can say to yourself, if you are a physicist: all right, I am simply going to neglect the ones I don't like because there are so few of them in comparison to the others. However, nothing can be done to the very last term in (55), because it simply does not change at all. No matter what you do with this model, the last term simply insists on staying. No symmetrization will help you -- nothing will help you except to simply forbid terms like this. You can think of it as follows: If $C_{12\ldots n}$ were sizable then my initial distribution would have a lot of this extraordinarily high harmonic component. It would be an extremely wiggly thing. If

you think of an ordinary Fourier series, where for instance a coefficient of a very high harmonic, say 10,000, is sizable then that means that you have components in the curve of frequency 10,000. It is terribly wiggly, so that you have to know the curve with great precision over very small time intervals. That's the Fourier's series case. In this case, I must simply assume that $\rho(\vec{\eta}, 0)$ is a relatively smooth function; that is, I cannot allow my initial distribution to be too fine-grained. In particular, I would not be allowed to start with all the balls black. That's too sharp, and the $C_{12\cdots n}$ coefficient is simply one. In fact, all of the coefficients are one.

So, I must first of all, assume that $\rho(\vec{\eta}, 0)$ is smooth so that I can neglect the last coefficient and others like it. Secondly, I must symmetrize. Even then I still have a problem. Because there are a lot of terms in equation (55), and even though in each individual term I am throwing away only a small proportion of the members, it could be that the cumulative error I am going to make is going to hurt me. Actually, I'm not even sure on this model whether I can show this or not. In the physical literature, where one tries to imitate this for the real Liouville equation for a gas, all that is done, and not even that quite precisely, is to show that in the few early terms the error is of small order. Whether or not they will accumulate is difficult to say.

On the other hand, you can say to yourself that I'm not going to be so ambitious as to justify the full Master equation. Rather, I'm going to stick to physical statements about single particles, pairs of particles, or triples of particles. Don't forget that the Master equation gives you a description of the whole statistics of all the sites of particles. If I am only going to ask questions which will never involve correlations or joint distributions of

more than three particles, then, of course, I will never go beyond the triple product of the η's. The neglect of the terms which don't decay will then be of course perfectly justified.

Consequently, this already sheds some light on how far we should trust the Master equation. We certainly ought not to trust it when it comes to conclusions involving numbers of particles comparable to the total number. But presumably you may as well accept everything else. So we may replace our deterministic model -- you might call it a deterministic model with final averaging-- by a stochastic one.

There are still various inconveniences involved. We may have to deal with infinite matrices, for instance. Because really, if you want to be a mathematician, you would have to perform the limit $n \to \infty$. But then you have an infinite matrix and the purely mathematical nuisances become very cumbersome to deal with. So close your eyes to it a little bit, and simply keep n fixed. But consider t small compared to n -- for instance, you allow t to go as far as the square root of n. I will postpone further discussion of these points until I come to the Boltzmann equation where the same difficulty arises.

This model has been useful to us. On it you have seen in excruciating detail essentially all the difficulties, all the problems and all the approaches that one uses in the kinetic theory of non-equilibrium phenomena. It perhaps looked a little more formidable than it really was, because the formulas were so long. I will now see what can be done by honestly assuming from the very beginning what you might call a stochastic model. Let me first say a few introductory words. In classical physics -- (that's discounting quantum mechanics where there are various added features) -- the use of probability is twofold.

There are some theories which, from the very beginning, cry out for a probability model. Without ever saying why or without bothering to justify it, one simply makes an assumption that the process under consideration is what we will call a random process. One then proceeds with an analysis of that. Examples of such problems would be Brownian motion, noise in electrical circuits, and similar problems. In all of these you are willing to accept a stochastic model from the very beginning.

On the other hand, there is a much larger and older body of physical theory -- revolving, roughly speaking, around kinetic theory and statistical mechanics -- where the use of probability theory has to be justified. In fact the old masters of the game, primarily Boltzmann, felt very uncomfortable about using probability. Even now, the majority of physicists, when faced with matters involving gases or liquids, are very reluctant to use it. They will tell you that there must be some way in which they can treat it purely dynamically.

In the example which I discussed at such great length I have tried to show you at least that it's possible to justify a probability model. Except that even when this is done, there still remains this necessity of averaging. In every probabilistic model in physics and in all other sciences there must be some lack of specification over which you can average. In the example I considered it was the set S. That's the whole problem as to how probability can be introduced in kinetic theories of mechanics. It's not completely solved yet; it's in a state of flux. But what I would like to show you is that at least as far as the theory of the ideal gas is concerned, the most elementary portion of Boltzmann's work can be put into a probabilistic scheme quite consistently. In just the same way we wrote out the Master equation for our model, we can also

write a Master equation for an ideal gas. We can then study it as a mathematical entity and see whether conclusions we derive from it do or do not agree with the standard conclusions of other theories. This point of view leads to a variety of problems both mathematical and physical. Some of the mathematical problems, remarkably enough, have not been properly settled. Some of them are of a very curious nature which I will discuss with you, where progress really would be of considerable and fundamental interest, I think.