ENTROPY—A DIALOGUE

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A scientist who worked all his life in field theory but was always very curious about entropy, an emotional topic among some of his colleagues, dies and is ushered into a very large room. There, behind a desk, sits an old angel. On the desk and on the shelves lining the walls are many books and instruments — some familiar, some strange. The eye of the scientist (S) is attracted to a shiny sphere with some special aura surrounding it. After some exchange of pleasantries with the angel (A) he asks what is inside the sphere.

A: The sphere is filled with one heavenly mole (2^{81}) of very small hard balls: they occupy a volume fraction 2^{-18} of the outer ball which has a volume of 1 cubic meter. These particles move according to Hamiltonian dynamics with elastic collisions and are perfectly shielded from *all* external influences. I started them a very very long time ago in a particular microscopic state X, which I picked at "random" from a region Ω of the phase space; the phase points in Ω correspond to all the particles being (without overlap) inside a ball with the same origin and one tenth the radius of the big ball, with a total energy (all kinetic) between $E \pm \Delta E$, E corresponding to average speed of 10^5 m/sec and $\Delta E = 2^{-18}E$. I have watched them evolve since then out of curiosity for how such a classical system would behave.

This is great, thinks S. Here is my chance to find out about entropy but I better check first if there is any trick here.

S: How interesting. I assume that your computers, I mean brains, are big enough and accurate enough so that you know the exact position and velocity of each particle at every

instant of time.

A: Yes, of course.

S: But then you also know in advance how it will evolve. Why do you bother with this experiment?

A: You see, while I (and other angels of my category) have essentially unlimited memory and therefore can have perfect knowledge of the past and present state of the system, I do not have any special computational abilities and therefore am unable to predict the future any better than mortals are. It is therefore fun to watch these particles evolve in accordance with Newtonian dynamics. In fact I think of it as an analog computer.

S: OK, so please let us discuss it. According to my understanding the initial time evolution should have been described very accurately on the mesoscopic level by the Boltzmann equation (BE). This should lead to a spatially uniform state with a Maxwellian distribution of velocities in a relatively short time. Since then I imagine the system has been in equilibrium with small fluctuations which are quite well described by the linearized BE with Gaussian noise .

A: Absolutely. That is exactly how it evolved on the mesoscopic scale.

S: Fine, but let me ask you: are you really sure that your system is truly isolated?

A: Yes. Just for fun I occasionally exactly reverse all the velocities and let the system evolve for a few years and then reverse the velocities again. The particles all retrace their trajectories perfectly. Actually doing that is not cost free — decreasing the entropy always requires some effort.

S: So I guess you can make them all return to their initial state but have you ever seen

them all go back spontaneously into the little ball where you started them from?

A: Oh, you mean a Poincaré recurrence. Actually yes, I have witnessed such an event once but don't really expect to see it again. I will surely be replaced here by another angel much before then.

S: And just before that return how did the entropy of this isolated system behave?

A: That was the most interesting part. Suddenly for no apparent reason it just kept decreasing until it was back to where it started at the beginning and then after a brief time interval it started increasing again as if nothing special happened.

S: But what about the second law? You have actually seen it violated. So it is not an absolute law. This is exactly what caused the heated lunch time discussions in our cafeteria.

A: Sure. Isn't that exactly what Maxwell, Boltzmann and Gibbs clearly said. All you have to do is wait long enough and have your system well isolated. These are both things that come naturally to me — remember I am older than your universe by quite a bit which, by the way, is why I am into this classical business. But enough of me, you look puzzled.

S: Yes, I am puzzled. To help clarify it for me, let me ask you what is the present entropy of this system?

A: Looking at it at this instant it seems to be in a typical equilibrium configuration, pretty uniform spatially with a Maxwellian distribution of velocities. Hence the macrostate is the equilibrium one. So if you want the value of the entropy, just take the log of the phase space volume appropriate to its energy, and get the value given in the textbooks.

S: This is what has been puzzling me for a long time. According to the textbook this is the

entropy appropriate for ignorant mortals who have to use some phase space probability density μ. Given such a μ they compute the entropy via $-\int \mu \log \mu \, dX$; this formula, first introduced by Gibbs and later extended by Shannon and others, has been almost synonymous with entropy in our world. You on the other hand know the microscopic state, so your probability density is in effect a delta function, why shouldn't then your entropy be $-\infty$? Or, if you use some discretization to take into account quantum mechanics or whatever, then it should be zero. Why should the volume of the energy surface be relevant for you?

A: Oh, but I was not talking for anybody in particular. Of course I do know, to any precision I care, the exact locations and velocities of the particles. I thought you were asking me about the present macrostate corresponding to the energy and density profile of the system and how many microstates, i.e., phase space volume, fit in it. Obviously, no matter what we really know, this quantity is unambiguously defined, up to relatively negligible terms which depend on the precision with which you define your macrostate, and it gives rise to the standard entropy.

S: What do you mean by standard entropy? Are there different entropies?

A: Well of course. Not only are there different types of entropy that are useful for different types of problems but within many of these you have still differences depending on what relevant macrovariables you take. There is the measure-theoretic entropy, the topological entropy, the von Neumann entropy, the Gibbs entropy, the H-functional, the Clausius thermodynamic entropy, the Boltzmann entropy, etc.

S: I have always felt that it is unfortunate to have so many quantities with the same name

but what are you talking about in the present context.

A: Here we are speaking in a statistical mechanical context and I was referring to the Boltzmann entropy and also to the thermodynamic equilibrium entropy. You must know that these are only defined once you specify the macrovariables. So if you give me another set of macrovariables, you get a different Boltzmann entropy.

S: But is this choice completely arbitrary?

A: Yes and no, it depends for what purposes you are going to use this entropy. If you want to use it as a predictive tool for the time evolution, as in the second law, then it is closely linked with the type and level of description you are using. Actually for the gas in this ball you could usefully compute it from the one particle distribution function as in the kinetic theory of gases. The Boltzmann equation will then describe the way it changes (except of course in some very special cases, like the ones we discussed earlier). So you see you are free but certain choices make much more sense. In fact, for thermodynamics I would even say you have a rather limited choice.

S: Then what determines a good choice.

A: What you are really asking is what makes a function on the microstate a good macrovariable. One thing that is crucial is to have a function that is additive. The reason is that then most of phase space, say corresponding to a given energy, is occupied by one very large region where these macrovariables are constant. It also helps to use quantities which are conserved locally. This essentially selects the energy, momentum and particle number.

S: How do you measure these volumes in phase space?

A: You count. It is a bit tricky but you can for all practical purposes also take some nice

density over which you integrate.

S: Then what would be an example of having different entropies in your sense?

A: There are many but here is a trivial one. Suppose that I have here red and green particles and that initially, all red particles were on the right side of my ball and all green particles were to the left. Same pressures, same temperatures. Now I let them go and they mix. I get something brown. Did the entropy increase?

S: This I know. Of course the entropy increases. I can even compute by how much.

A: Aha, but now suppose that you were colorblind, you could not see the difference between green and red and you would see something pretty uniformly grey from beginning to end.

S: And the particles can be assumed to be individually taking each exactly the same paths as before?

A: Yes. The microscopic dynamics is identical.

S: Strange. Now I would say there is no increase in entropy. Is that not related to the Gibbs paradox?

A: Indeed, as is its solution. You see, there are many entropies. In one case you add the extra macrovariable giving you both the color and density-profile but if you don't care about color you just inspect the overall density profile.

S: There is one thing I am now confused about. If there are these different entropies corresponding to what you and I decide to include as macrovariables, how can the measurement of entropy be objective, yielding the same result for all of us?

A: That is a good question. The solution is that you should think about what is relevant and what is not for the problem you are considering. The possibility of having different

entropies is not at all harmful as long as you understand that it corresponds to different situations, e.g. are you interested in properties of the system which depend on the color of the particles or not? Of course in the former case you better have someone or some instrument which is color sensitive.

S: Do you mean something like contextual?

A: Something like that but don't make it too complicated. Just imagine a colorblind man trying to sort out green from red particles. As for contextuality, you also have it in quantum mechanics. Maybe it is to this that you refer.

This is an opportunity to ask about quantum statistics, feels the scientist. And who knows, perhaps the angel will tell me some quantum secrets.

S: That reminds me. As you know everything, is there still something like indistinguishability for you?

A: No, I can distinguish all particles.

S: That is what I thought but then how do you get quantum statistics and why do you divide by this $N!$ in front of the Liouville measure?

A: Now it is me not understanding your question.

S: I have seen many textbooks arguing for extensivity of the entropy via quantum mechanics and I have learnt that quantum particles follow a Bose-Einstein or Fermi-Dirac statistics for their occupation numbers. But they must be indistinguishable.

A: Did that not sound a bit strange to you?

S: No no, it looked pretty convincing.

A: But they did not know about me, it seems. The problem of extensivity of entropy is

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unchanged in going from classical to quantum physics.

S: Are you saying that this indistinguishability is similar to your example of colorblindless where you can exchange red for green?

A: It is. You see, also classical particles with the same charge, mass and what have you, don't come equipped with distinguishing labels. They are in fact only distinguished by their dynamic properties. That is the history of their momenta and positions. There is no reason therefore to be mystical about this $N!$; it emerges naturally in classical mechanics just like in quantum mechanics.

S: Perhaps so but, at any rate, quantum mechanics is much more complicated. Since there is no obvious quantum phase space of microstates there is also no obvious phase space volume so tell me, how should one define the quantum Boltzmann entropy?

A: Boltzmann speaks about the connection between the microscopic and macroscopic thermal properties of physical systems. This can be divided into two parts. The first part gives a microscopic formula for computing the entropy $S_B(M)$ of a macroscopic system specified to be in a macrostate M, e.g. one described by the hydrodynamic variables entering the Navier-Stokes equation. This goes over without any deep conceptual problems to quantum mechanics. Given M you can still use Boltzmann's formula $S_B(M) = k \log |\hat{\Gamma}(M)|$ where $|\hat{\Gamma}(M)|$ is now the dimension of the linear subset of the Hilbert space of the system corresponding to M. This makes sense because the variables defining the macrostate, e.g. those specifying (to some appropriate accuracy) the particle number, the momentum and the energy in each macroscopically small but microscopically large region of the volume occupied by the system, can be chosen to essentially commute and so they form an orthogonal

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decomposition of the Hilbert space.

S: That's great. I actually remember reading about that in von Neumann's book but had forgotten about it since all the textbooks and papers always use for the entropy the formula $-kTr(\hat{\mu}\log\hat{\mu})$ where $\hat{\mu}$ is the density matrix but that is zero if you are in the pure state Ψ.

A: Yes. This quantum version of the Gibbs entropy, also called the von Neumann entropy, has produced even more confusion than its classical counterpart. But aside from this unnecessary confusion you, I mean your colleagues still down there, do have a real problem when it comes to the second part of Boltzmann's micro-macro connection. Given a point X in the phase space we always have a well defined M: call it $M(X)$. This defines the Boltzmann entropy $S_B(X) = S_B(M(X))$ for a single macroscopic system like the hard spheres inside this box. As you know, this is important for giving a clear microscopic interpretation to the second law. There is no such relationship between Ψ and M for quantum systems: the wavefunction of the system does not necessarily specify a unique macrostate. Think of Schrödinger's cat.

S: That is exactly what I was just thinking about. How can I understand this?

The angel shakes his wings and thinks, here is somebody who in fact wants to understand quantum mechanics.

A: Well, to tell you the truth I don't really understand it either. I think that there are other ways to think about quantum mechanics but I am not really the right angel to explain them. Why don't you see my colleague Angel Psi.

S: Good. I want to see Angel Psi. I have many questions for him.

A: I wish you good luck.

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