On the Microscopic Origin of Macroscopic Phenomena[1]

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Science is the human endeavor to understand the nature of the world into which we are born. This quest for understanding is driven by practical needs as well as by an innate curiosity which, whatever its evolutionary origin and utility, goes far beyond the utilitarian. Even very young children have this basic urge to explore and examine. When maintained into adulthood it gives rise to all human creativity including that in the sciences, both theoretical and experimental.

I belong to the theoretical physics community. My main interest is in finding out how the dynamics of the microscopic components of matter, such as atoms and molecules, determine the behavior of macroscopic objects containing very many atoms, objects that we can see and touch, like a glass of water or a piece of metal. This is the subject of statistical mechanics which provides a mathematical framework for describing how well-organized higher level structures or behavior may result from the random, nondirected activity of a very large number of interacting lower level entities. Fortunately, an understanding of many aspects of the behavior of macroscopic systems—such as the boiling and freezing of water—can be obtained from simplified models of the structure and interaction of atoms. We can often take as our starting point Feynman's description of atoms as "little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another". (The degree to which this simple picture gives predictions which are not only qualitatively correct but in many cases also highly accurate, is remarkable, since the structure of real atoms

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is governed by quantum mechanics and is much more complicated than Feynman's rather crude classical picture.)

Statistical mechanics explains how macroscopic phenomena originate in the cooperative behavior of these "little particles". Some of these phenomena are simply the effects of the combined actions of many individual atoms; for instance, the pressure exerted by a gas on the walls of its container is due to the continual bombardment of the walls by very many gas molecules. But other phenomena are examples of emergent behavior; they have no direct counterpart in the properties or dynamics of individual atoms. Particularly fascinating and important examples of such emergent phenomena are (1) the irreversible approach to equilibrium and (2) phase transitions in equilibrium. Both of these would be astonishing if they were not so familiar. Their microscopic understanding and analysis form the core of my own research. Let me sketch them very briefly.

The problem of irreversibility can be stated as follows. Most of the processes we can observe going on in the world about us are *uni-directional* or *asymmetrical in time*. They display an *arrow of time*: cooked vegetables cannot be uncooked, splattered eggs do not reassemble. Yet this manifest fact of our experience is particularly difficult to explain in terms of the fundamental laws of physics. Newton's laws, quantum mechanics, electromagnetism, Einstein's theory of gravity, etc., make no distinction between the past and the future—they are *time-symmetric* and completely reversible. It is only the secondary laws, those that describe the behavior of macroscopic objects containing many, many atoms, which explicitly contain time asymmetry.

A prime example is the second law of thermodynamics which states that an isolated macroscopic system evolves uni-directionally in time towards equilibrium—a state characterized by the maximization of a quantity called *entropy*. (The entropy of a macroscopic system is a measure of the number of microscopic states in which the system can find itself at a given energy or temperature—it can therefore also be thought of as a measure of disorder, suitably defined.) The explanation of why and how such time-asymmetric macroscopic behavior arises from completely reversible microscopic dynamics is well understood in principle: it is due to the universe starting out in a state of very low entropy. The current problems concern the derivations and solutions of equations describing these phenomena quantitatively.

The second example of emergent phenomena, much investigated by statistical mechanics, is that of phase transitions in equilibrium systems, such as occur in the boiling or freezing of water. Here dramatic changes in structure and behavior of the macroscopic system are brought about by small changes in the temperature or pressure without any change in the structure of the individual atoms or molecules making up the system. For example the volume occupied by a kilogram of water molecules at atmospheric pressure, while changing only very little when the temperature increase is between 5^oC and 95^oC, increases by a very large factor when the temperature changes from 99.9999^oC to 100.0001^oC. Even more dramatic things happen in the freezing transition around 0^oC where there are essentially "infinite" changes in some properties, like fluidity. For more details see items 370, 383 and 434 in the publication list on my web site: http://www.math.rutgers.edu/~lebowitz.

Please look also at the Human Rights page on my web site. I believe that scientists have special responsibilities in this area. The scientific perspective makes differences between people based on nationality, race, religious belief or gender entirely trivial, while making the things humans have in common, such as the potential to comprehend many aspects of our universe, very special and significant. The scientific outlook should therefore make scientists work hard for a sustainable and just world.