BROKEN SYMMETRY, EMERGENT PROPERTIES, DISSIPATIVE STRUCTURES, LIFE: ARE THEY RELATED?

by

P. W. Anderson ‡ * and D. L. Stein

Princeton University **

The more theoretical physicists penetrate the ultimate secrets of the microscopic nature of the universe, the more the grand design seems to be one of ultimate simplicity and ultimate symmetry. Since all of the interesting parts of the universe - at least those of interest to us like our own bodies - are markedly complex and *unsymmetric*, the first, correct conclusion one draws from this statement is that the deep probing of the nature of matter (on which physicists expend great effort and greater sums of money) is becoming more and more irrelevant to *us*. But that isn't really an adequate retreat for any scientist who hopes to achieve the ultimate goal of science, which we take to be real understanding of the nature of the world around him from first principles. It is essential for him to explain the real world in terms of the ultimately simpler constituents of which it is made. In fact, he must thank his stars that the world becomes simpler as each underlying level is discovered - the opposite case would make his task difficult indeed.

The simplicity to which we refer is, of course, the recent success of the elementary particle theorists in reducing the equations of the fundamental constituents of matter to perfectly symmetrical ones, in which all constituents initially enter in exactly the same way, and in which all the interactions themselves are derived from a principle which *itself* is a manifestation of an especially perfect kind of symmetry. But those who are not acquainted with these developments need have no fear that what we say will depend on them in any way. we wish merely to make the point that there is a sharp and accurate analogy between the breaking-up of this

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* Also at Bell Laboratories, Murray Hill, New Jersey 07974.

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ultimate symmetry to give the complex spectrum of interactions and particles we actually know, and the more visible complexities we will shortly discuss.

There has been gradually arising during the past twenty years or so a set of concepts related to the ways in which complexity in nature can arise from simplicity, some of which are quite rigorously and soundly based in the theoretical physics of large and complex systems, while others extend all the way to the speculative fringe between physics and philosophy.

The most basic question with which such a conceptual structure might hope to deal would be placing life itself within the context of physics in some meaningful way: to relate the emergence of life itself from inanimate matter to some general principle of physics. Can we understand the existence or even the origin of life in some purely physical context?

We approach this question in four steps. Clearly, we are trying to look at life as what the philosophers call an *emergent property:* a property of a complex system which is not contained in its parts. So we start from the very simple question of whether such properties exist at all.

The most rigorously based, physics-oriented description of the growth of complexity out of simplicity is called the theory of *broken symmetry.*

> Can properties emerge from a more complex system which are not present in the simpler substrate from which the complex system is formed?

The theory of broken symmetry gives an unequivocal "yes" answer to this question: In equilibrium systems containing large numbers of atoms, new properties - such as rigidity or superconductivity - and new stable entities or structures - such as quantized vortex lines - can emerge which are not just nonexistent but meaningless on the atomic level.

Unfortunately, the emergent properties we are most seriously interested in are not these simple ones of *equilibrium* systems: specifically, we need to know whether life, and then consciousness, can arise from inanimate matter, and the one unequivocal thing we know about life is that it always dissipates energy and creates entropy in order to maintain its structure. So we come to a second deep question:

> Are there emergent properties in dissipative systems driven far from equilibrium?

The answer is yes: dynamic instabilities such as turbulence and convection are common in nature and their source is well-understood mathematically. When they occur these phenomena exhibit striking broken symmetry effects which very much resemble the equilibrium structures which exist in condensed matter systems. These have been called "dissipative structures". Examples are convection cells or vortices in turbulent fluids. But these seem always very unstable and transitory: can they explain life, which is very stable and permanent (at least on atomic time scales)?

> Is there a theory of *dissipative structures* comparable to that of equilibrium structures, explaining the existence of new, stable properties and entities in such systems?

Contrary to statements in a number of books and articles in this field, we believe there is *no such theory* and it may even be that there are no such structures as they are implied to exist by Prigogine, Haken and their *collaborators*.[1,2] What does exist in this field is rather different from Prigogine's speculations and is the subject of intense experimental and theoretical investigation at this time.

Thus the answer to the fourth deep question

> Can we see our way clear to a physical theory of the origin of life which follows these general lines?

is already evident: No, because there exists no theory of dissipative structures. The best extant theoretical speculations about the origin of life, those of *Eigen*[3], are only tenuously related to the idea of dissipative structures, and instead are sui generis to the structure of living matter; still, it may be that they contain deep problems of the same sort which destroy the conventional ideas about dissipative structures. We are setting out to study this question in detail.

The above is the basic outline of what we have to say: now we would like to set it all out in more specific and detailed terms.

Initially, we must learn some things about the real physics: What and why is "broken symmetry"? - more properly called "spontaneously broken symmetry". The answers to both questions are so simple that we almost miss their depth and generality. First, what is it? Space has many symmetries - it is isotropic, homogeneous, and unaware of the sign of time, at the very least. Correspondingly, the equations which control the behavior of all particles and systems of particles moving in space have all of these symmetries. But Nature is not symmetric: "*Nature abhors symmetry.*" Most phases of matter are unsymmetric: the crystals of which all rocks are made, for instance, are neither homogeneous nor isotropic, as Dr. Johnson forcefully pointed out. Molecular liquids are often not *isotropic* but form liquid crystals (see Fig. 1); magnets such as iron or rust (which is antiferromagnetic) are not invariant under time-reversal. Superfluids break one of the hidden symmetries of matter, the so-called gauge symmetry, allowing the phase of quantum wave-functions to be arbitrary, related to the laws of conservation of charge and number of particles.

Second, why? Fluctuations, quantum or classical, favor symmetry: gases and liquids are homogeneous, magnets at high temperatures lose their magnetism. Potential energy, on the other hand, always prefers special arrangements: atoms like to be at specific distances from each other; spins like to be parallel or antiparallel, etc. Thus we define *spontaneously broken*

Definition. Although the equations describing the state of a natural system are symmetric, the state itself is *not*, because the unsymmetric state can become unstable toward the formation of special relationships among the atoms, molecules, or electrons it consists of.

So far the idea is purely descriptive: it becomes meaningful when we find that it relates and explains many apparently different and unrelated phenomena. Initially, the concept was introduced by *Landau*[4] to solve a series of problems related to the nature and meaning of thermodynamic phase transitions, but it also relates and explains many other properties of broken symmetry phases. In the course of this, he introduced the single most important concept of the whole theory: the idea of the *order parameter*.

The order parameter is a *quantitative measure* of the loss of symmetry. The canonical one is $\vec{M}$ in a ferromagnet: the mean moment $<\mu_i>$ on a given atom. Others are:

1. director $\vec{D}$ of the nematic liquid crystal;
2. amplitude ρ_G of the density wave in a crystal;
3. mean pair field in a superconductor $<\psi\ (r)>$.

Landau: *the loss of symmetry requires a new thermodynamic parameter whose value is zero in the symmetric phase* - for instance, the magnetization of a ferromagnet (see Fig. 2), the director in a nematic liquid crystal, etc. The magnitude of the order parameter η measures the degree of broken symmetry.

This has many implications. For instance, the appearance of a wholly new thermodynamic variable is a necessary condition for a continuous (so-called second-order) phase transition. It can, and often does, appear discontinuously, but it need not - see M(T) in Fig. 2, and for contrast ρ_G (T) in Fig. 3 for a typical crystal. Also, since there is an extra parameter, the free energy and all the thermodynamic properties can never be the same mathematical functions in the two phases of different symmetry, so the phases are always separated by a sharp phase transition - unlike, for instance, water and steam.

The thermodynamic consequences which flow from the amplitude of η alone are ample excuse for the broken symmetry concept - but even more important consequences follow from another property of the order parameter which Landau never formalized but sometimes used *it is a quantity which always has a phase: the free energy $F\ (\ T, |\eta|\ )$ is a function of its magnitude $|\eta|$*

but must not be so of its "phase" or direction, because of the existence of the original symmetry. For instance, the energy may not depend on the *direction* of the director since space is isotropic; nor may it depend on the orientation or position of a crystal, nor on the phase ϕ, of the superfluid wave function. Another way to say it is that the order parameter has a space within which it is free to move without changing the energy. (In quantum-mechanical terminology, the ground state is highly degenerate in the broken symmetric phase, which in a way is a remnant of the original symmetry of the Hamiltonian (which remains unchanged). This is connected to some of the dynamical consequences of broken symmetry, such as Goldstone modes and the Higgs phenomenon, as will be shortly discussed.)

A second property of η is obvious if we see it as a physical thermodynamic parameter: it may vary over macroscopic distances in the sample, and $\eta(r)$ may be defined locally (just as we can define a *local* temperature or pressure in a sample not too far from equilibrium, if these do not vary too rapidly.)

From this follow three major emergent properties of spontaneously broken symmetry:

1. Generalized rigidity
2. New dynamics
3. Order parameter singularities and their role in dissipative processes.

All of these are very interesting, since most of the important properties of solids depend upon them, but time and our subject mean that we can only afford to discuss the first, which is the simplest and most general.

Again we use the idea that η is a physical thermodynamic parameter to which we can by one means or another apply a force. This is clear in the case of $\vec{D}$ - which couples to boundary orientation - or of $\vec{M}$ or crystal orientation θ , ϕ; but it can be a little more w esoteric for "hidden" order parameters like sublattice magnetization in the antiferromagnet or ψ the superfluid order parameter. Nonetheless it is always possible to grasp hold of η at any point in the system. While F is not a function of the phase angles of η, it is naturally a function of the *gradient* of these phases, because otherwise arbitrarily large relative fluctuations of the phase would destroy the existence of the order parameter. Thus we must have

$$F = F(|\eta|, |\nabla\eta|^2, \ldots)$$

and

$$\frac{\partial^2 F}{\partial(\nabla\eta)^2} > 0$$

a positive stiffness for variations of η.

This is enough to ensure that if we exert a force on η (r) at *one* end of a sample, $\eta(r')$ will respond at the other. We can essentially use η as a crankshaft to transmit forces from one point to another, that is, to exert action at a distance (see Fig. 4). We emphasize that this rigidity is a true *emergent property:* none of the forces between actual particles are capable of action at a distance. It implies that the two ends cannot be decoupled completely without destroying the molecular order over a whole region between them.

Rigidity of solids, then, is a model for a wide class of other rigidity properties, including permanent magnetism, ferroelectricity, and superconductivity and superfluidity. These last two have, since the discovery of the Josephson effect, been understood to be the phase rigidity of the order parameter $\psi(r)$[5].

The other two major emergent properties are also consequences of this phase freedom in broken symmetry systems: the existence of long-wavelength collective motions of the order parameter, such as phonons and spin waves, which are the models for the Goldstone and Higgs phenomena of elementary particle physics; and the existence and classification of singularities and textures of the order parameter: the possible order parameter fields which are allowed when we permit lower-dimensional regions to be excluded from our order parameter field $\eta(r)$ - vortex lines and dislocations, domain boundaries, singular points, etc. Broken symmetry gives rise to the appearance of new length scales that did not exist in the symmetric phase.

Now let us return to the main theme of our discussion: that there does *not* exist a corresponding theory of the dissipative case. First, let us describe the kinds of experiments which seem at first to lead to very similar types of broken symmetry in the dissipative case and have been so described. The canonical example is the Bénard instability: the layer of fluid heated from below, which, once a critical heating rate is exceeded, exhibits very regular-appearing "rolls" of convection, arising spontaneously with a rather fixed size or wavelength (see Fig. 5).

Other examples abound, such as the Couette instability of a viscous fluid between rotating cylinders (Fig. 6), or even the familiar laser exhibiting a periodic wave of excitation density (Fig. 7).

Clearly all of these systems exhibit spontaneously broken symmetry in the simple sense, in that, for instance, in each case the sign is arbitrary, and also an initially homogeneous state changes suddenly into an inhomogeneous one. The initial transition is often continuous, just like the typical second-order transition, and it has often been suggested that there is some kind of deep analogy between these two types of systems. There is indeed one mathematical respect in which there is at least a similarity, in that both are examples of dynamic instabilities, for which there exists a general mathematical theory described by *Thom*[6] called "catastrophe theory" and much elaborated in recent years by a large number of mathematicians of whom perhaps *Ruelle*[7] should be specially cited. But the thermodynamic phase transitions invariably present only the simplest kind of catastrophe, the so-called "bifurcation", and the simplest type of state, the so-called "fixed point", while dynamical instabilities seem always to evolve, - even oversimplified mathematical models of them - towards more and more complex types leading eventually to completely chaotic behavior. The evolution of chaos in such systems has been beautifully described by *Gollub*[8] in a number of articles and by R. Abrahams and J. *Marsden*[9] in a well-known book. It is a pity that I cannot describe here in detail the beautiful work described in these sources in following the successive instabilities from classical to steady rolls to singly-periodic dynamic to multiply periodic and finally to total chaos.

Experimentally the situation is even more complex. *Ahlers*[10] particularly has shown that even the complicated behavior seen by *Gollub*[8] and predicted by the mathematicians may be an artifact of an over-constrained system heavily influenced by its boundary conditions: they find finer-scale chaos or near-chaos even in the apparently quiescent region of the Bénard system We have tried to show that this is inevitable and that dissipative structures in a real, physical, open system unconstrained by artificial boundary conditions will inevitably be chaotic and *unstable*[11,12]. (For instance, the laser can be persuaded to oscillate in a single mode only with the utmost artificiality and difficulty. This depends on the proper placement of endplates or mirrors so that here broken symmetry is strongly dependent on externally applied boundary conditions. Lasers occurring naturally in nature (for example, from astrophysical sources) seem to show no mode selection.)

Prigogine and his school have made a series of attempts to build an analogy between these systems and the Landau free energy and its dependence on an order parameter, which leads to the important properties of equilibrium broken symmetry systems. The attempt is to generalize the principle of maximum entropy production which holds near equilibrium in steady state dissipative systems, and to find some kind of dissipation function whose extremum determines the state. As far as we can see, in the few cases in which this idea can be given concrete meaning, it is simply incorrect. In any case, it is clearly out of context in relation to the observed chaotic behavior of real dissipative systems.

Thus we conclude that there is no analogy visible between the stability, rigidity and other emergent properties of equilibrium broken symmetry systems, and the properties of dissipative systems driven far from equilibrium. The latter types of systems have never been observed to, nor can any mathematical reason be found why they should, exhibit the rigidity, stability, and permanence which characterizes the thermodynamically stable broken symmetry systems. (A case in point of a driven system that might have exhibited broken symmetry but failed to do so is described ~~in Refs. 11 and 12~~.)

The reason this is unfortunate is that many authors have chosen to use such systems as the laser and the Bénard instability as models for the nature and origin of life itself, as an emergent property of inanimate matter. It is indeed an obvious fact, noted since Schrödinger's 1940 *book*[9], that life succeeds in maintaining its stability and integrity, and the identity of its genetic material, at the cost of increasing the rate of entropy production of the world as a whole. It is at least in that sense a stable "dissipative structure" - i.e., an existence proof by example.

Turing[14] long ago observed that a fertile source of dynamic instabilities was the autocatalytic chemical reaction in which reaction products serve as catalysts as well. The base-pairing mechanism of DNA is an obvious and good example. *Eigen*[3] in particular has tried to develop a theory of autocatalytic instabilities in the primeval soup as a detailed explanation of the origin of life. It is a glorious picture to imagine the growth of an "order parameter in molecular information space," driven by a dynamic autocatalytic instability and self-stabilized in some mystic way by the magical power of Darwinian evolution. This may in fact be the way it happened - one can hardly assume it did not! - but there are reasons to be skeptical of the claim that we have yet found the full story. Why should dynamic *instability* be the general rule in all other dissipative systems, except this supremely important one? We are attempting a computer simulation of a model of the origin of information-carrying macromolecules which is already producing quite interesting results in terms of the spontaneous generation of complex molecules. (See Appendix)

Let us then conclude by reiterating our main point: we still believe, since in fact we understand the process in all details, in the reality of emergent properties: the ability of complex physical systems to exhibit properties unrelated to those of their constituents. But we do not believe that stable "dissipative structures" maintained by dynamic driving forces can be shown to exist in any inanimate system, and thus we do not see how speculations about such structures and their broken symmetry can yet be relevant to the still open question of the origin and nature of life.

Appendix

In the simple picture we are using, we begin with a 'soup' of monomers of two different varieties, A and B, and an externally applied energy flux which drives the system toward formation of strings of monomers, according to a simple set of rules for lengthening and shortening chains. This process relies on temperature cycling: in the low temperature phase two strands (or a strand and monomers) attach weakly via A-B attraction (as in hydrogen bonding between a purine-pyrimidine pair). While held together in this fashion, stronger bonding may take place between two adjacent, previously unattached strands. In the high temperature phase the hydrogen bonds break, but the stronger bonds along the length of the strands do not, and the newly created (or lengthened) strands separate until the next cycle. There is a slightly higher probability for strong bonding between dissimilar monomers than for similar ones. There is also a certain chance that, in the high temperature phase, a strong bond may be broken (and a strand thereby shortened) because of, say, interaction with an energetic cosmic ray. In addition to these 'birth' and 'death' rates (more accurately, lengthening and shortening processes) there is also a small error probability; that is, in the low-temperature phase, an A monomer may mistakenly hydrogen bond to another A, rather than a B as it should. These birth, death, and error rates thus form a complete prescription for building up many lengthy strands starting from a sea of lone monomers and a single strand of two or three monomers.

We wish to see if, from this very simple picture, a polymer with nontrivial information content will be selected from the near infinite number of possibilities, selection (if it exists) being implicit in the strong nonlinearity of the problem. Clearly, if most chains are of the form ABABABAB .... (or AAAAA... or BBBBB...) nothing very interesting has happened. On the other hand, if many chains with irregular sequences, such as ABBABABAAABBA... are formed but no pattern appears to predominate, again little of interest has occurred.

In looking for patterns that may predominate, we have found it most useful to search for 'triplets', by which we mean the following. Suppose we are given the strand that appears above:

$$A_2B \wr BAB_6ABA \wr A_1 \wr A_2B \wr B_2A$$

Whenever two like monomers appear adjacent, we draw squiggly lines separating them as pictured. We then count the respective lengths of the purely alternating sequences that make up the polymer (these are the numbers that appear in the picture above). A "triplet" is then the triplet of lengths of three adjacent alternating sequences; in the example above, we have a (2, 6, 1), (6, 1, 2), and (1, 2, 2). Note that the mirror image of the polymer would give the same result. We therefore wish to see if certain triplets make up the bulk of most long polymers. This seems to us to be more useful than trying to select an entire polymer itself as the prototype of what should be selected.

Our preliminary results indicate that for certain choices of bonding probabilities selection of a number of triplets occurs and can in fact be quite strong (as well as persistent over many cycles, which is a requirement if we are to say selection has occurred). It is also amusing, and somewhat unexpected, that a small error probability is necessary for selection to occur in the cases studied so far.

Many questions remain unanswered, the most prominent of which is, how does one assign a meaningful information content to a polymer? So far we've only discussed necessary, but not sufficient, conditions for symmetry breaking in "information space" to occur. One would guess that, in some sense, structure and function are intimately related (in that in the real world, DNA serves as a blueprint for manufacture of proteins, some of which act as enzymes in replication and other processes governing the DNA molecule itself). Is there any way in which this can be seen in the simple model presented here? This is one of the most fundamental problems in understanding the origin of life, a not so subtle variant of the "chicken and egg" *problem*[3]. We are not attempting to answer this problem at this stage, but rather the somewhat less ambitious problem of whether one can relate the issues of symmetry breaking discussed earlier to the problem of the origin of life (specifically, a primitive genetic code in this instance), and in what context this is possible and meaningful.

References

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FIGURE CAPTIONS

1a. Nematic liquid crystal in the disordered state. The line segments represent the rodlike molecules of the nematic. Averaging molecular orientations over macroscopic distances yields zero.

1b. For a suitable choice of thermodynamic parameters, the nematic enters the ordered state, with the appearance of a macroscopic order parameter (the director $\vec{D}$). The system is no longer isotropic, but has chosen a special direction: rotational symmetry has been broken.

2. Variation of magnetization M with temperature T in a simple ferromagnet. This is a typical second-order phase transition, in which the order parameter grows continuously from zero as T is lowered below a critical temperature T_c.

3. In a first-order transition, such as the liquid to solid crystal transition shown here, the order parameter will exhibit a discontinuous jump at the transition with an associated release (or absorption) of latent heat.

4. Illustration (somewhat schematic) of generalized rigidity. An external force (the crank) couples to the order parameter at one end of the system, represented as a gear. A change in the order parameter at any point in the

ordered system is transmitted to all other parts of the system (first gear turns the second gear). The second gear turns the second crank: a force has been transmitted from one end of the system to the other via the order parameter.

5. The Bénard instability in rectangular geometry. A layer of fluid between two horizontal rectangular plates is heated from below. When a sufficient thermal gradient is reached between top and bottom plates, convection arises in the form of rolls. In this cutaway edge-on view, the arrows represent the fluid velocity.

6. Couette flow: A fluid is placed between two cylinders with different rotational velocities about their axes. When the velocity gradient exceeds a critical value, rolls of vortices form. In this view the cylinder is cut along its length.

7. In a laser, a standing wave of excitation density is set up between two end plates, or mirrors, resulting in emission of a beam of coherent radiation.

1a

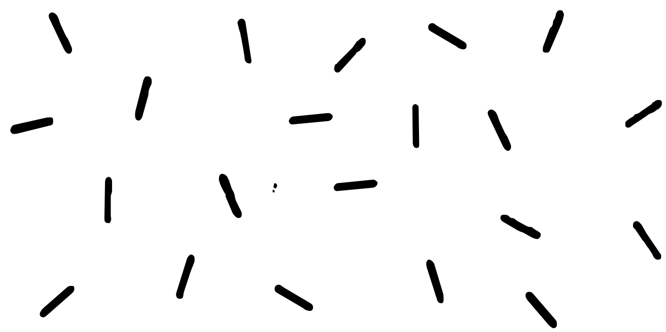

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Fig. 1a

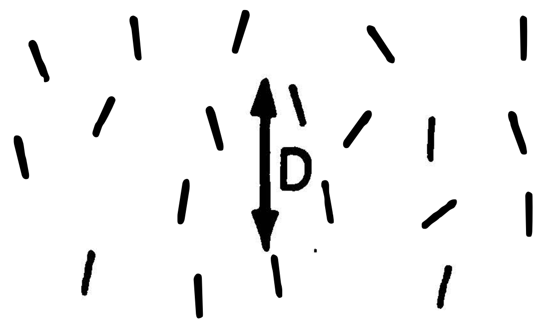

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Fig. 1b

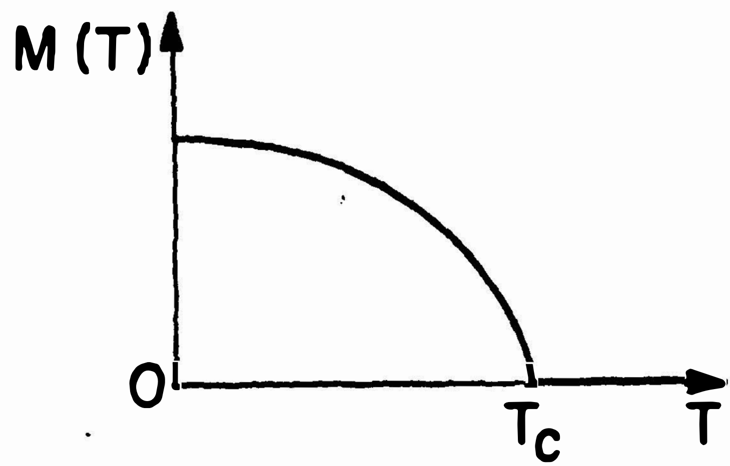

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Fig. 2

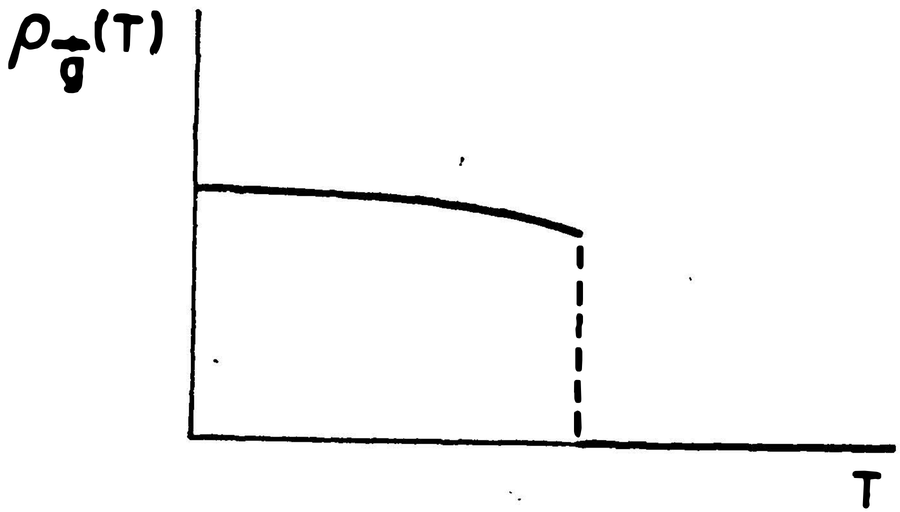

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Fig. 3

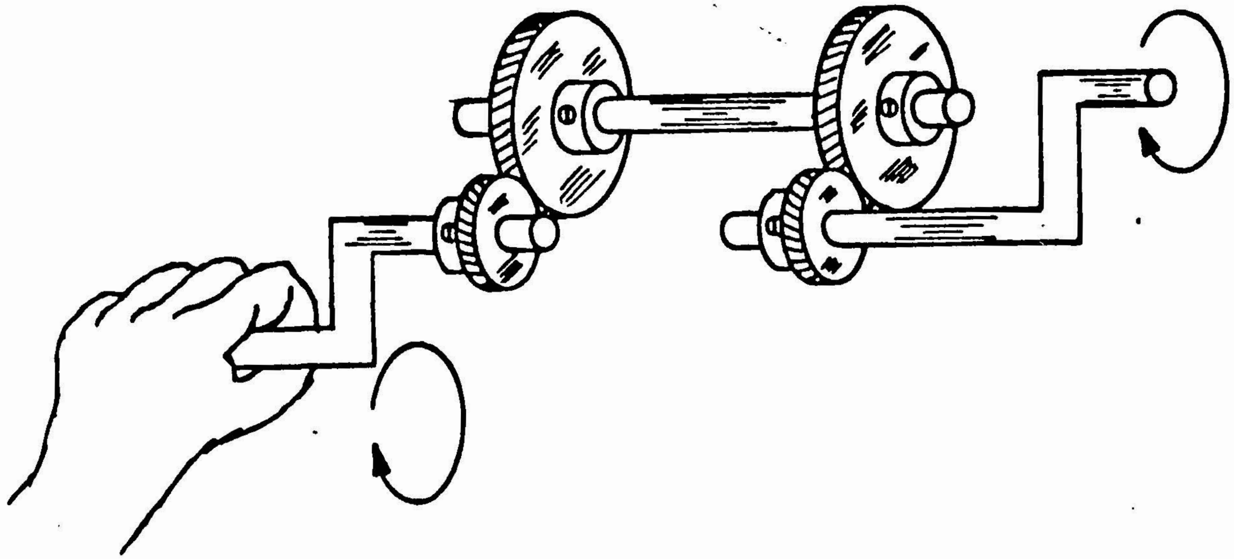

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Fig. 4

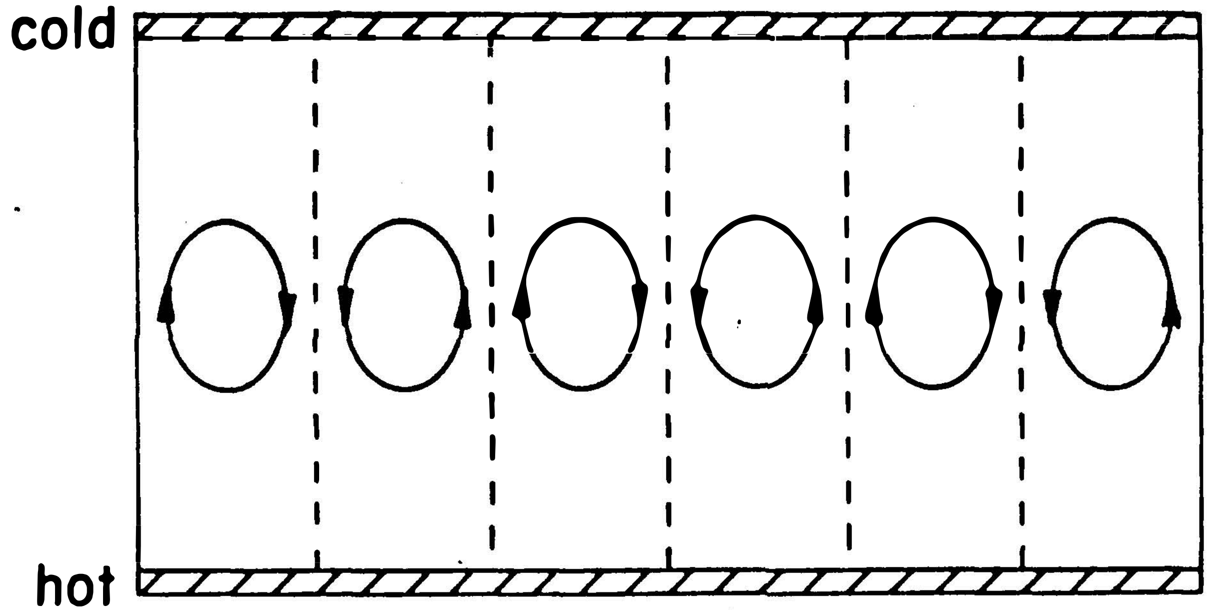

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Fig. 5

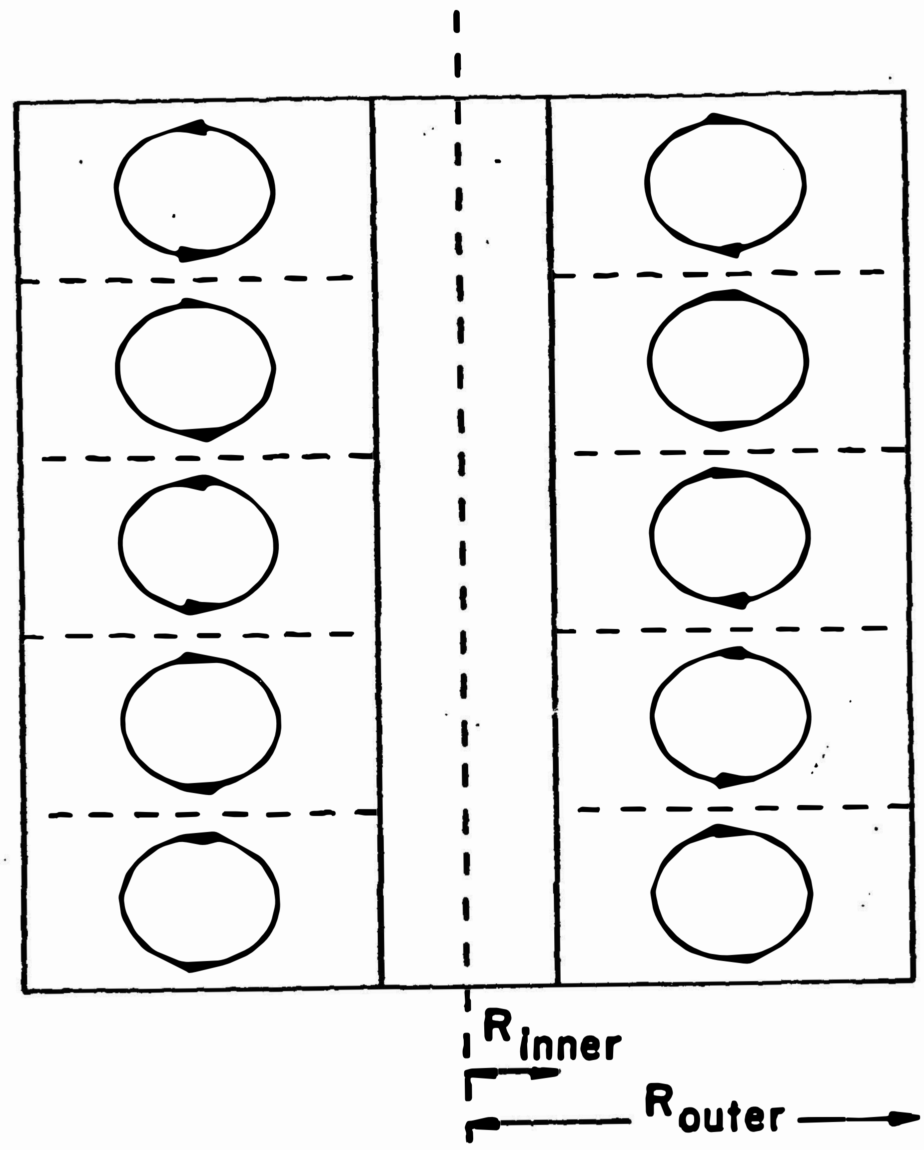

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Fig. 6

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Fig. 7