The Turing Instability as an Example of Non Equilibrium Symmetry Breaking

Abhishek Mukherjee
Department of Physics, University of Illinois at Urbana-Champaign,
1110 W. Green St., Urbana, IL 61801, U.S.A.
(Dated: December 13, 2005)

Abstract

The Turing instability has now been established as a canonical mechanism of stationary pattern formation both theoretically as well as experimentally. In this brief article the basic theory of this instability will be sketched, with special emphasis on the characteristics it has in common with symmetry breaking in equilibrium systems. A very brief introduction to some experimental and numerical results will also be given.

I. INTRODUCTION

In the year 1952 British mathematician Alan Turing made a remarkable prediction. From his mathematical model of chemical reactions he predicted that under suitable conditions chemical reactions may form *stationary* patterns in space. He claimed this to be the basis of *morphogenisis* i.e. the process of structure and pattern formation in the biological world [1]. This was certainly against the conventional wisdom of the time, according to which all systems being bound by the second law of thermodynamics necessarily evolve to spatially uniform states. However since then Turing's prediction (if not his claim) stands verified experimentally and strengthened theoretically.

The history of this acceptance is quite interesting. Chemical oscillations were observed for the first time the 1050's by Belosov [2]. Later, similarities with Turing patterns was noticed [22]. In the meantime the general theory of pattern formation was being developed from from different angles (from irreversible thermodynamics [3] to non linear dynamical systems). This made Turing's prediction theoretically much more plausible, however experimental proof still remained elusive until 1989, when for the first time Alan Turing's prediction was verified experimentally [4] (and references therein).

The basic idea behind Turing's prediction can be understood from the following set of equations [5].

$$\frac{\partial U}{\partial t} = D_U \nabla^2 U + f(U,V)$$
$$\frac{\partial V}{\partial t} = D_V \nabla^2 V + g(U,V)\ , \tag{1}$$

where U and V are the concentrations of the so called 'activators' and 'inhibitors' of describing a set of system of chemical reactions. It is assumed that the concentrations of any other chemical species which may be present is kept constant and is hence absorbed in the definitions of the various parameters. D_U and D_V are the diffusion constants for U and V respectively. Also, $f(U,V)$ and $g(U,V)$ are the reaction terms, which are in general non linear. They are derived from the law of mass action and the existing physical conditions. What Turing predicted is that under certain conditions the homogeneous solution (see later) to the above equations can become unstable against the formation of stationary patterns. A few interesting features of the Turing patterns are the following:

- The diffusion constants (D_U and D_V) should differ significantly in magnitude.
- The lengthscale of the patterns are instrinsic to the system.

In the next section we will very briefly review the general phenomenon of pattern formation in non equilibrium systems, in Section III we will try to get a theoretical understanding of the Turing patterns in this light. In Section IV we will have a brief look at the experimental situation, and finally we will conclude in Section V.

[22] It should be noted however that they are in principle quite different. Turing patterns are stationary while in the original BZ reactions travelling waves were produced.

II. SOME GENERAL CONCEPTS OF NON EQUILIBRIUM PATTERN FORMATION

The formation of structures and hence symmetry breaking is not unique to non equilibrium systems. They can be seen in equilibrium as well; examples would include crystals and ferromagnetism. In particular, the latter is often taken to be the canonical example of equilibrium critical phenomena and there exists a well developed language (order parameter, spontaneous symmetry breaking etc) and techniques (mean field theory, renormalisation group) of statistical thermodynamics for the analysis of such phenomena. These concepts are often profitably exported to their non equilibrium counterparts.

However there are certain very important caveats. In non equilibrium, interesting structures like the Turing patterns are often found in what are known as non equilibrium steady states. Operationally steady states can be defined as states with well defined long time (asymptotic) macroscopic averages in systems which are subjected to time independent boundary conditions. Typically non equilibrium steady states will have (constant) inflow and outflow of generalised fluxes (e.g. energy, matter etc.). This in general leads to violation of detailed balance and hence *prima facie* makes a ensemble based analysis diffcult. More importantly, perhaps, any kind of completely *macroscopic* phenomenology (thermodynamics) is hard to justify for such systems (see, however, [6]).

Let us consider an example. In the 1960's and 70's a thermodynamic description of systems far from equilibrium was formulated by Prigogine and others of the Brussels-Austin group[3]. This in turn was a generalisation of their thermodynamic theory of systems near equilibrium[7]. The basic principle that they proposed is that a form of generalised 'excess entropy production' (subject to constraints) is minimised in non equilibrium situations. Crudely speaking, in this theory spatial/temporal structures emerge when the homogeneous solution to the extremisation condition ceases to be stable (i.e. it becomes a maximum instead of a minimum). Since these strucures could be maintained far from equilibrium mainly due to the dissipation of the input energy, they were named *dissipative structures.*

The above is a representative example. There are numerous other approaches of similar nature(see in [8]). The central theme of all such formalisms seems to be an attempt to replace the detailed dynamics by an appropriate minimisation (maximisation) principle in the characterisation of locally stable states. In equilibrium statistical thermodynamics the same is done by minimising the free energy. In analogy a 'non equilibrium free energy' or in more technical terms a (local) Lyapunov function is sought. In a series of influential papers Landabuer pointed out that this is essentially equivalent to trying to calculate the relative occupation probabilities of different states of local stability from the local values of the functional without invoking the nature of the intervening sparsely occupied states [8]. He then argued (convincingly) that this is in general not possible for non equilibrium steady states, i.e. the transtion dyanamics between the locally stable states cannot be neglected [23].

After the rather unflattering comments of the previous paragraph, it should be noted that

[23] His argument essentially was that it is possible to change the transtion probabilities by creating temperature inhomogeneities far from the points of local stability. This will change the relative probability of the states with local stability but will not change the local structure of the Lyapunov functional. This counterintuitive proposal often called the *blowtorch theorem* has been confirmed from various model dependent

these 'thermodynamic' theories are not without value altogether. Historically they have been instrumental in providing an atleast intuitive justification of non equilibrium pattern formation from the thermodynamic perspective; in particular, they provided a simple explanation of why these structures are not incompatible with the second law of thermodynamics. Also, from the practical point of view they can be used to get a rough understanding of different features of non equilibrium structures. For more quantitative results however these rather qualitative insights should be augmented by microscopic and/or semi microscopic theories.

Now let us discuss some aspects of symmetry breaking in non equilibrium systems. It is without doubt that pattern formation is a result of symmetry breaking, as such they can be thought to be analogous to critical phenomena (second order phase transitions) in equilibrium statistical physics (or condensed matter physics). However, *almost twenty five years ago* Anderson argued that this analogy is probably a superficial one [10]. In condensed matter systems, (spontaneous) symmetry breaking is most interesting when a continuous symmetry is broken (e.g. the Heisenberg model of a magnet). In that case broken symmetry or Broken Symmetry, in Anderson's notation, is associated with a number of other universal phenomena. These include

- low energy excitations with no restoring force, i.e. the Goldstone modes
- generalised rigidity
- topological defects which relax generalised rigidity.

He claims (and rightly so) that there exists (at that time) no evidence of such phenomenon for the non equilibrium symmetry breaking. In the next section we will discuss Anderson's criteria for Turing systems [24].

III. THE BASIC THEORY OF TURING INSTABILITY

As we have already mentioned generic Turing systems are modelled by Eq. 1. To get a qualitative understanding let us first consider the linear theory. The homogeneous solution, $U = U_0, V = V_0$ to Eq. 1 is given by the zeroes of the reaction terms $f(U, V)$ and $g(U, V)$

$$f(U_0, V_0) = 0 = g(U_0, V_0) \tag{2}$$

Now consider a small peturbation(u, v) about this solution.

$$u(x, t) = \sum u_j e^{\lambda_j t - k_j x} \tag{3}$$

$$v(x, t) = \sum v_j e^{\lambda_j t - k_j x} \tag{4}$$

calculations [9].

[24] For examples of each of these phenomena in other non equilibrium systems please see [11].

Note that x and k_j's are the coordinates and wavevectors, respectively, in any dimension, i.e. they are vectors. Now, let us define the matrix $\mathbf{A}$ by,

$$\mathbf{A} = \begin{pmatrix} \partial_U f & \partial_V f \\ \partial_U g & \partial_V g \end{pmatrix}_{(U=U_0, V=V_0)} \tag{5}$$

Similarly the diffusion matrix, $\mathbf{D}$, is defined by,

$$\mathbf{D} = \begin{pmatrix} D_U & 0 \\ 0 & D_V \end{pmatrix} \tag{6}$$

The eigenvalues λ_j's can be found by solving the following characteristic equation

$$|\mathbf{A} - \mathbf{D}k_j^2 - \lambda_j \mathbf{I}| = 0 \tag{7}$$

All modes with $\mathrm{Re}(\lambda(k)) > 0$ are unstable. However Turing patterns are stationary patterns, i.e. for the Turing instability $\mathrm{Im}(\lambda(k)) = 0$. This fact can be used to determine the critical wave number (k_c) at the bifurcation point. At the bifurcation point $\lambda(k_c) = 0$. This, when substituted in Eq 7 (and combined with the fact that there are no unstable modes without diffusion i.e. $\mathrm{Re}\lambda(k) < 0 \ \forall k$ when $\mathbf{D} \equiv 0$) gives the following solution for k_c at the bifurcation point,

$$k_c^2 = \frac{D_V f_U + D_U g_V}{2 D_U D_V} \tag{8}$$

Above the bifurcation point (threshold) there will in general be a range of wave vectors which will become unstable. These wave vectors will be bounded on the above and below by, say k_- and k_+, such that $\lambda(k_{\pm}) = 0$. Hence $k_{\pm}$ are given by,

$$k_{\pm} = \frac{D_V f_U + D_U g_V}{2 D_U D_V} \pm \sqrt{\frac{f_U g_V - f_V g_U}{D_U D_V}} \tag{9}$$

As a rule of the thumb the width of this range($|k_+ - k_-|$) increases with the distance from threshold. However in contradistinction to order-disorder equilibrium phase transitions the Turing instability itself remains stable only over a range of the parameters. The conditions for the existence of the generic Turing instability are,

$$f_U + g_V < 0 \tag{10}$$

$$f_U g_V - f_V g_U > 0 \tag{11}$$

$$D_V f_U + D_U f_V > 0 \ . \tag{12}$$

From the above relations it can be shown that $D_U \neq D_V$, i.e. the difference in diffusion coefficients is crucial for the Turing instability to occur as advertised [25].

[25] This (Turing) instability should be carefully distinguished from the closely related Hoft instability, which happens when the uniform solution becomes unstable with respect to (temporal) limit cycles, $\mathrm{I}m\lambda(k_c) \neq 0$. The intercation between Turing and Hoft instabilities can give rise to interesting phenomenon, but that is beyond the scope of our discussion.

It should be clarified that the linear theory is only a crude indicator of the various instabilities that can take place. A more complete theory should take into account the various nonlinearities of the problem atleast in the form of controlled approximations. In general this is practical only in certain domains. [11]

- Near the bifurcation point (threshold). Here the nonlinearities are small, and the variations (spatial and temporal) of the patterns are slow. The (coarse grained) equations governing these variations, the so called 'amplitude equations' are generally of a few *universal* forms (governed by the symmetry of the problem). This approach has very strong analogies with the Landau theory of equilibrium phase transitions. For a more complete treatment one needs to take into do this more carefully, i.e. one needs to take into account the renormalisation corrections. However as a matter of experience it has been seen that the 'critical region' for these systems are typically very small, hence mean field theory seems to be a very good description, even very near the threshold.

- Small distortions from regular patterns (far away from the threshold). These can also be treated perturbatively with what are called 'phase equations' which also some in certain universal forms.

The key technique used in the both the above mentioned cases is that of elimination of the 'fast modes' (which are expected to follow the dynamics of the 'slow modes' adiabatically). This is called the 'slaving' of 'fast modes' [12]. Near the threshold both the amplitude of the (marginally) unstable modes as well as the phases of the associated symmetry modes are the slow modes. However far from the threshold the amplitudes relax very fast, only the phases remain as the slow modes. I will briefly mention some of these detailed techniques and their results in the next section.

For now, let us discuss a slightly more coarse grained and hence more universal description of the problem. Let $A(\mathbf{x}, t)$ be the amplitude of a slow mode, mentioned above(A is a complex field). Then atleast near the threshold the evolution equation for A (with suitable rescaling) can be very well approximated by [11],

$$\frac{\partial A}{\partial t} = \epsilon A + D\nabla^2 A - g_0 \left|A\right|^2 A \; . \tag{13}$$

Note that A can be regarded as the order parameter (density) for the system. One can immediately write a Lyapunov functional for the above equation

$$\mathcal{L} = \int d\mathbf{x}(-\epsilon \left|A\right|^2 + D \left|\boldsymbol{\nabla}\right|^2 + g_0 \left|A\right|^4) \tag{14}$$

such that Eq. 13 can be written as

$$\frac{\partial A}{\partial t} = \frac{\delta \mathcal{L}}{\delta A^*} \tag{15}$$

The analogy with equilibrium (Landau) free energy functional in Eq.14 is evident. In this light D should be interpreted as the generalised rigidity which is responsible for long range forces.

Notice that Eq. 13 is invariant under constant phase shifts of A, this merely reflects the fact that nothing changes if the whole pattern is given a constant translation. Now consider smooth long wavelength phase modulation of A , say $\delta\Phi = \delta\Phi_0 \cos(Qx)$ $(Q \ll \epsilon)$. We can see that the relaxation time for this mode is , $\tau \sim Q^{-2}$, i.e. with a large enough wavelength the relaxation time can be made arbitarily large. These long wavelength modes should be thought of as the 'Goldstone modes' for this system.

Finally, let us notice that phase fluctuations of the above form and small amplitude fluctuations, it can be shown that the amplitude fluctuations will adiabatically follow the phase fluctuations, as such the generic phase equation (with rescaling) can be extracted as the Kuramoto-Shivashinsky equation [13],

$$\frac{\partial \Phi}{\partial t} = -\nabla^2\Phi + \alpha\nabla^4\Phi - \mu(\boldsymbol{\nabla}\Phi)^2 \tag{16}$$

It is well known that patterns generated by Eq.16 exhibit defects, which can be treated as the non equilibrium analogues of topological defects found in equilibrium ordered phases which relax generalised rigidity (The equation itself actually holds good even well into the broken symmetry phase.).

IV. RESULTS FROM DETAILED CACULATIONS, SIMULATIONS AND EXPERIMENTS

A. Theory

The actual task of eliminating the fast modes and finding the slow modes can be carried out in a few different ways. One method which is often used is called the multiscale method. In this method the appropriate bifurcation parameter (i.e. the parameter which measures the distance from the threshold) and the concentrations are expanded about a small parameter. For example, if a be the bifurcation parameter and a_c be its threshold value then we can expand [5]

$$a - a_c = \epsilon a_1 + \epsilon^2 a_2 + \cdots \tag{17}$$

The equations for the various modes now become linear differential equations. The coefficients for the coarse grained amplitude (phase) are determined from the solvability conditions of these equations.

Another method which is frequently used for such analysis is called the center manifold reduction. The basis of this method is the center manifold theorem. Crudely, the center manifold states that there exists a critical manifold for the non linear system which is locally tangential to the critical manifold of the linear theory ($\lambda(k) = 0$), such that trajectories in its neighbourhood converge exponentially (in time) on it [26]. What this means is that most of the interesting nonlinear effects, atleast near bifurcation points, is effectively confined to a lower dimensional space, as conpared to the full dynamics whose phase space can in principle be infinite dimensional (one for each legitimate wave vector). This should be compared with the 'slaving' principle mentioned earlier. The center manifold reduction for the Turing system has been done by [19]. We will briefly discuss their results later.

[26] Note that the center manifold theorem is an existence theorem, not an uniqueness theorem. But as with most such cases in physics uniqueness is only justified *a posteriori*.

Other than the above mentioned analytical techniques, Turing systems (like most non linear systems) are extensively studied using numerical and computational techniques, and in most cases they are very useful not only quantitatively but also in unravelling the qualitative features especially in the region of the parameter space between the two limits mentioned earlier, which is inaccessable to analytical tools.

I will not go into any further technical details of the nonlinear theory, but will merely state the commonly accepted results of the same. Eq. 1 is the generic model for reaction diffusion systems in general, but in order to study Turing pattern formation in specific systems, the forms of f and g must be specified. This leads to various specific models ; the commonly used ones being the Brusselator model [14], the Gray Scott (GS) model [15], the Lengyel-Epstein (LE) model [16], and the more recent BVAM model [17]. The patterns show model dependent features, but certain universal features can also be seen.

In one dimension the only patterns which are possible are one dimensional lamella. However one interesting feature is that the presence of a constant source term in Eq. 1 changes the transition from a sharp one to a more smeared one and also brings about hysterisis effects. This is however not peculiar to Turing systems only but is a common feature in most nonlinear systems [11]. In two dimensions however more interesting patterns are formed. This case has been studied extensively both anaytically and numerically. The robust patterns which are seen are spots and stripes. A common feature which emerges is that the presence of *quadratic* terms (like UV) favors the formation of spots, while the presence of *cubic* terms (like UV^2) favours the formation stripes. Typically when both the terms are present these two patterns compete until one is selected depending on the relative strength of the two terms. If stripes are selected then it seems that they asymptotically settle down to a pattern of straight stripes. In case the spots are selected they typically settle down to a hexagonal lattice, although square and pentagonal lattices (wih defects) are also possible under certain special conditions [18].

The three dimensional case is much richer. Analytical calculation using the Brusselator and the LG models show that lattices of spherical droplets with simple cubic, FCC, BCC and double diamond symmetry are stable in different regions of the paramter space, as are lamella [19]. However numerical simulations with the BVAM model suggests that the situation may be more complicated. Unlike in two dimensions where in a given parameter range only one pattern dominates asymptotically, that may not be the case in three dimensions. Structures which are observed correspond to something between lamella and droplets, also the packing of the droplets is not a simple cubic, FCC or BCC but can be a mixture of them [5]. The model independent features in three dimensions are still not clear.

B. Experiments

Until quite recently attempts to observe Turing patterns experimentally proved unsuccessful. A key reason for this reason is the fact that the Turing patterns are *diffusion driven*, they require the diffusion constants to differ significantly. Experimentally this is a challenge because typically almost all small molecules have similar diffusion constants ($\sim 10^{-5}cm^2$/s). This was the case in some of the more common reactions which exhibited chemical pattern formation like the Belousov-Zhabotinsky (BZ) reaction.

The first unambiguous experimental verification of the Turing pattern in a chemical system was obtained by De Kepper's group at Bordeaux in 1989, some forty years after Turing's original paper [20]. This reaction generally goes under the name the chlorite-iodide-maloric acid-starch (CIMA) reaction. Ironically the most important roadblock was cleared almost by accident. De Kepper's group were studying oscillations in the chlorine dioxide-iodine-maloric acid (CDIMA) reaction. They added *starch* merely to improve the colour contrast. However, in addition, starch also to iodine to form starch-triiodide complex, which reduced the mobility of the iodide ions and thereby enhanced the ratio of the diffusion constants between iodide and chloride ions. Turing patterns were obtained with respect to iodide and chloride concentrations. The following observations proved conclusively that the observed patterns were Turing patterns.

- The symmetry breaking did not take place in the direction imposed by the feeding gradients.
- A gel strip near the feeding inlet prevented any convective motion, thus this was purely a reaction diffusion process.
- The patterns remained stationary as long as the system parameters (feeding rates) remained stationary.
- The lengthscale of the pattern ($\simeq 0.2mm$) was different from any externally imposed lengthscale and seemed to be an intrinsic lengthscale of the system.

Also the patterns were reproducible and relatively robust against perturbations (e.g. intense light).

Similar observations were made by other groups and Turing like patterns were reported in various other systems including ecology, fluid dynamics, semiconductors, astrophysics etc. [4]. Interestingly recently Turing patterns were observed in a slight modification of the BZ reaction (the BZ-AOT reaction) [21]. These experiments have served to verify the existence of the patterns, so far no detailed quantitative comparison of theory and experiment has been attempted. Also, although there have been attempts to explain biological pattern formation in terms of Turing pattern, there is as yet no conclusive evidence for the same.

V. CONCLUSION

In this essay, some the universal features of stationary non equilibrium pattern formation were discussed, using the Turing instability as a canonical example. Particular emphasis was placed on the features which these phenomena share with equilibrium phase transitions. Very little could be said about properties which seem to be peculiar to non equilibrium structures (as opposed to equilibrium) in general and Turing patterns in particular, due to the limited scope of this article. The overall discussion was rather heuristic and only the features exhibited by 'generic' Turing patterns were discussed, none of the specific model dependent features were discussed. Most of what has been described in Section III roughly corresponds to what is called mean field theory in the case of critical phenomena. We have not discussed any corrections to this mean field theory, that can in principle come from renormalisation. Also we have not discussed, at all, the effects of noise which turn out to be very important for non equilibrium systems.

In conclusion it should be mentioned that Turing's original claim that biological patterns are formed due to stationary diffusion driven instabilities is far from being confirmed, it is still a highly controversial topic. However as it often happens in scientific enquiry, his idea has found homes is various diverse unexpected systems. Today it serves as a major paradigm in the characterisation and analysis of pattern formation far from equilibrium.

---

[1] A.M. Turing, Philos. Trans. R. Soc. London Ser. B **2**37, 37 (1952)

[2] B. P. Beluzov, in *Oscillations and Travelling Waves in Chemical Systems*, ed. R.J. Field and M. Burger, Wiley, New York, 1985, p. 605

[3] G. Nicolis and I. Prigogine Self Organization in Non-Equilibrium Systems, 1977, Wiley

[4] P.K. Maini, K.J. Painter, H.N.P. Chau J. Chem. Soc., Faraday Trans. **9**7, 3601 (1997)

[5] T. Leppanen, in *Current Topics in Physics* ed. R. A. Barrio and K. Kaski, Imperial College Press, 2004 and references therein

[6] Y. Oono and M. Paniconi, Progr. Theo. Phys. Suppl. **1**30, 29 (1998), S. Sasa and H. Tasaki, cond-mat/0411052

[7] G. Nicolis, Rep. Prog. Phys. **4**2, 225 (1979)

[8] R. Landauer, Phys. Rev A, **1**2, 636 and references therein

[9] S. Fekade and M. Belake, Eur. Phys. J. B, **2**6, 369 (2002)

[10] P.W. Anderson, in *Order and Fluctuations in equilibrium and Non Equilibrium Statistical Mechanics* ed. G. Nicolis, G. Dewel, J.W. Turner, Wiley, 1981, p. 289

[11] M.C. Hohenberg and P.C. Hohenberg, Rev. Mod. Phys., **6**5, 851(1993)

[12] H. Haken, Rev. Mod. Phys., **4**7, 67 (1975)

[13] G. Nicolis, J. Phys. Condens. Matter, **2**, SA47 (1990)

[14] I. Prigogine and G. Nicolis, J. Chem. Phys. **4**6, 3542 (1967)

[15] P. Gray and S.K. Scott, J. Chem. Phys. **8**9, 22 (1985) and references therein

[16] I. Lengyel and I.R. Epstein, Science, **2**51, 650(1991)

[17] R.A. Barrio, C. Varea, J.L. Aragon, P.K. Maini, Bull. Math. Biol. **6**1, 483 (1999)

[18] J.L. Aragon, M. Torres, D. Gil, R.A. Barrio, P.K. Maini, Phys. Rev. E **6**5, 051913 (2002)

[19] T.K. Callahan and E. Knobloch, Physica D, **1**32, 339 (1999)

[20] V. Castets, E. Dulos, J. Boissonade, P. De Kepper, Phys. Rev. Lett **6**4, 2953 (1990)

[21] V.K. Vanag and I. R. Epstein, Phys. Rev. Lett, **9**2, 128301(2004)