

# **This I understood in the Seminars**

Atul Singh Arora

*E-mail address:* to.AtulArora@gmail.com

*URL:* [http://www.github.com/toAtulArora/IISER\\_repo/](http://www.github.com/toAtulArora/IISER_repo/)

ABSTRACT. Seminars have been very challenging for me as the protocol of asking questions there is not very clear. Consequently, what follows, is not even close to being rigorous; the ideas understood, however have been attempted to be conveyed with enough clarity, although this may not represent my best work. The template used here is that of a book, however the chapters are merely corresponding to different seminars.

## Contents

Chapter 1. Adventures of the interface of physics, chemistry, biology and engineering	4
1.1. The facts	4
1.2. What I could follow	4
Chapter 2. A theoretical study of formation of clusters at nanoscale using reaction-diffusion models in one and two dimensions	6
2.1. The Facts	6
2.2. What I could note	6
Chapter 3. Coherences, Photosynthesis and Quantum Biology	10
3.1. The Facts	10
3.2. What I could partially follow	10
Chapter 4. Mechanics of Information Processing and Computation in Cells	14
4.1. The Facts	14
4.2. What I could follow	14

## CHAPTER 1

# Adventures of the interface of physics, chemistry, biology and engineering

### 1.1. The facts

**When, where and who.** The seminar was held on October 23, 2013, 4:00 PM, in LH 3 (LHC). The speaker was Prof. Deepak Mathur (TIFR, Mumbai).

**The Abstract.** Access to ultra-short laser pulses that last long enough to accommodate only a few optical cycles, is beginning to allow time dependent nuclear and electron dynamics to be probed within atoms and molecules, thereby enhancing our ability to gain proper insights into how quantum systems react to strong external fields and how they might be subjected to optical control. In this talk I shall present an overview of how we have utilized intense laser pulses of duration as short as 4 femto seconds to explore dynamical effects of relevance to diverse areas of the natural and engineering sciences, including application pertaining to DNA damage, laser-induced materials modification and green photonics.

### 1.2. What I could follow

Prof. Mathur started with talking about how very short duration of light pulses (order of femto seconds) allows only one or two wavelengths of light to fit in. He then talked about the intensity of his high energy laser.

To get an understanding of the strength of this laser, consider the hydrogen atom for instance. Its coulomb attraction force, is a result of the electric field which is given by

$$I = 2 \frac{\epsilon_0}{\mu_0}^{\frac{1}{2}} |E|$$

With  $E = 5 \times 10^9 V/cm$ , we get  $I = 3.5 \times 10^{16} W/cm^2$ .

He then talked about small disturbances in the hydrogen atom that can be approximated as a spring.  $F = -kz$ , where as for large enough disturbances you get terms of higher order as well, which add overtones of the oscillation frequency to the mix. He said theoretically because of this and the time dependence, large disturbances (produced by the laser in this case), this is a difficult problem to solve.

He considered the potential energy curve for a hydrogen atom given by

$$V = -\frac{q}{x} \pm E.x$$

which has roughly an energy  $10^{13} - 10^{14} W/cm^2$ . When this potential is distorted by the disturbance, there can be a situation where tunnelling occurs (roughly  $10^{14} - 10^{15} W/cm^2$ ) and then there can be a situation where it's over the barrier.

There was also then, a discussion on Pondermotive forces, which are given by

$$F_p = -\frac{e^2}{4m_e\omega^2}\nabla\langle E^2(x)\rangle$$

(which he mentioned is also there in Landau's book) and the potential for the same is then given by

$$U_p = \frac{e^2 I \lambda^2}{16c^2 \pi^2 m_e}$$

where  $I = 10^{16} \text{ W/cm}^2$ ,  $\lambda = 806 \text{ nm}$ ,  $U_p \sim 100 \text{ eV}$  so then we have  $U_p > \text{Interaction Energy} > h\nu$

Thereafter, he started discussing the effect of the laser on Ethanol. The experiments were performed on a single molecule, using techniques he said he'll mention later. The objective was to be able to break some specific bond, and not the one with the least energy first, and so on, as was thermodynamically predicted. To partially achieve this, he'd experimented with various polarizations of light, specifically linear and circularly polarized light. He was able to demonstrate that for the same intensity, the polarized light was able to break bonds much more easily. Further, he also showed that the thermodynamically expected behaviour of weaker bonds breaking first and the stronger linearly later, is not observed.

Next he talked studies related to how for a given carrier Gaussian envelope, changing the phase affects the action of light on the molecule. He went on to talk about how the duration of the pulse also plays an interesting role. He showed results of an experiment where a  $10 \text{ fs}$  laser beam produces mostly molecular entities, suggesting only the electronic degrees of freedom are affected by the pulse, as the nuclear degree of freedom operates in the time scales of roughly  $30 \text{ fs}$ . In an experiment with a  $30 \text{ fs}$  pulse, mixed entities were found (both atomic and molecular). However another experiment proved that in shorter time scales, these degree of freedoms actually combine. The experiment is related to the *Jahn-Teller Effect*. The consequence of this is that symmetric molecules like  $\text{TMS}^+$  can't quite be converted into  $\text{TMS}^+$ . However, as it turns out, using the laser method, one can produce these species which live for  $\mu\text{s}$ , by reducing the duration of the pulse to about  $5 \text{ fs}$ .

Due to shortage of time, Prof. Mathur screamed past numerous slides to reach the one that read Blood, Saliva and DNA. Their relevance here may seem to be absent, but he connected this by first talking about rivers and how dead bodies tend to end up on the river bank, even when carefully thrown at the centre of the banks. The point was that since the velocity of the central part of the flow is the highest, this is bound to happen. Now it gets interesting. This flow may be thought to depict the flow of blood in our vessels, and yet cells like the RBCs for instance, don't end up on the wall. The cause for this may be understood by one of the experiments performed by Prof. Mathur's group, which involved optically trapping (also known as optical tweezing in Biology) a single cell by virtue of creation of a potential minima using lasers, and then observe a fluorescent spot inside the RBC. The results of this experiment seemed to suggest that there's an uplift, like that produced by helicopters. This to a certain extent explains why the RBCs don't end up at the edges of the vessels. However, there seemed to be a lack of clear explanation to the claim, which was pointed out during the question answer session which followed.

## CHAPTER 2

# A theoretical study of formation of clusters at nanoscale using reaction-diffusion models in one and two dimensions

### 2.1. The Facts

**When, where and who.** The seminar was held on October 24, 2013, 3:00 PM, in LH 3 (LHC). The speaker was Dr. Trilochan Bagarti (Harishchandra Research Institute, Allahabad).

**The Abstract.** Nano-patterning on surfaces can be achieved by self-organization or artificially by direct atom manipulation. Surface defects plays a very important role in the formation of patterns at nano-scale. It has been observed in experiments that preferential nucleation of self-organized nano-structures takes place on surfaces along step edges, dislocations and domain boundaries. In the deposition of Ge atoms on Si(111)-(7x7) surface, we have found interesting patterns induced by domain boundaries and step edges. To understand the formation of these defects induced nano-patterns we have proposed a coupled reaction-diffusion equation in the presence of surface defects. I will discuss a linear model which qualitatively explains the experimentally observed pattern. Then I will discuss non-linear model which incorporates the effect of exclusion on these reaction diffusion processes. The effect of exclusion on simple trapping problem has been found to affect the stretched exponential behaviour of the asymptotic survival probability. This has been recently verified by our numerical simulation.

### 2.2. What I could note

The talk given by Dr. Trilochan Bagarti was rather inaccessible to our feeble minds. However, what I could understand to the most extend, was the contents of the first slide, the *outline*.

- (1) Motivation
- (2) Patterns in nature
- (3) Pattern formation in reaction diffusion systems (turing mechanism)
- (4) Reaction-diffusion systems in disordered media
- (5) Models
  - (a) Reaction diffusion models for formation of clusters on a surface with defects

He said that the motivation was lack of clear enough explanation of the formation of patterns on diffusion of Ge on Si(111)-(7x7). Patterns at a nano-scale seem to self organize. This can also be done artificially by atomic manipulation. He showed an STM image of a clean Si(111)-7x7 surface, where bilayer steps and terraces with

domain boundaries could be seen. The key ingredient necessary for the emergence of pattern from a uniform structureless state, he said, was instability that results in spontaneous breaking of symmetry.

There was a mechanism discovered by Alan Turing that talked about the origin of diffusion driven instabilities that can give rise to such patterns.

To solve this problem, he started with Linear Stability Analysis.<sup>1</sup> A homogeneous steady state solution to this may be given by

$$\dot{u}(t) = \rho(u(t)), u(0) = u_0$$

So we linearise  $u = u_s + \partial u$ ;  $\partial u \sim e^{\omega t + i k x}$  and solve the characteristic equation

$$\det(\omega I + |k|^2 D - J) = 0$$

where  $J$  is the Jacobian.

Then he turned to the Turing activator; inhibition model. For this he defined

$$n = 2, d = 2, u = (u_1, u_2)^T, \rho(u(t)) = (f, g)^T$$

$$D_{ij} = \delta_{ij} D_i \quad i, j = 1, 2 \quad D_1, D_2 > 0 \text{ and const}$$

$$\omega_1 \omega_2 < 0 \text{ using the characteristic equation}$$

$$K^4 - \alpha^2 \left( \frac{\partial u_1 f}{D_1} + \frac{\partial u_2 g}{D_2} \right) + \left( \frac{\partial u_1 f \partial u_2 g - \partial u_2 f \partial u_1 g}{D_1 D_2} \right) < 0$$

Turing space

$$\frac{\partial u_1 f}{D_1} + \frac{\partial u_2 g}{D_2} > 0$$

$$\left( \frac{\partial u_1 f}{D_1} + \frac{\partial u_2 g}{D_2} \right)^2 - 4 \left( \frac{\partial u_1 f \partial u_2 g - \partial u_2 f \partial u_1 g}{D_1 D_2} \right) > 0$$

Next he discussed models of diffusion on disordered media and also in regular lattice. He further showed simulations of Sierpinski Gasket and Percolation Cluster. He talked about anomalous diffusion in some detail.

$$\langle R_N^2 \rangle = N^{2/d\omega}$$

where

$$d\omega = 2 - d - d_f = 2.32 \pm 0.01$$

He then talked about fractal dimensions, stating  $p$  = fraction of occupied states and at  $p = p_c = 0.592745$  (transition).  $p < p_c$  would imply only finite clusters and  $p > p_c$  implied only large infinite clusters.

Next he talked about a random walker that walks after waiting a time  $\tau$ , continuous time random walk.

$$\psi(\tau) \sim \tau_0^4 t^{-1-\mu}$$

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<sup>1</sup>I must mention that the mathematical formulations weren't very accessible to me, for lack of understanding of certain mathematical tools. However, I was able to note down some of the equations, which may be useful in some way.

This was followed by a discussion which had a few more pictures; *Trapping reaction-diffusion problem*. Diffusing particles arriving at the traps get annihilated. This is given by

$$A + T \rightarrow (1 - \epsilon)A + T$$

So the probability in the case where the traps are distributed uniformly, and are static, we obtain

$$p(t) \sim e^{\alpha_d \rho^{2/(d+2)} t^{d/(d+2)}}$$

And for the case of mobile traps we have

$$p(t) \sim \begin{cases} e^{-\alpha_1 \rho t^{1/2}} & d = 1 \\ e^{-\alpha_2 \rho t / \ln t} & d = 2 \\ e^{-\alpha_3 \rho t} & d = 3 \end{cases}$$

This work was done by Balagurov & vaks, Donsker and Vardhan & Bramson, Lebowitz, Bray and others.

If you take a distribution of traps, there'll be large regions where there're no traps. Consequently there'll be particles that take a very long time to get trapped. Further, there's no recent work, in which they have fully modelled moving traps.

He next talked about solving for such a 1 D system, using the *Green's Function Method*. Assuming the trapping reaction to be in 1D, we have  $\delta = \{x_1, x_2, \dots, x_n, \dots\}$  uniformly distributed in  $\mathbb{R}$ , we have

$$\partial_t U(x, t) = \nabla \partial_x^2 U(x, t) - k \sum \partial(x - x_i) \mu(x, t) \text{ where } x \in \mathbb{R}, t > 0$$

Then, he talked about *perfect traps and the law of stretched exponential*. The mathematical parts of this have been skipped as the notes weren't consistent. The idea however was that every particle that arrives at the trap vanishes. In this case, the x-axis becomes a collection of disjoint intervals. He then showed that here, the survival probability, the lengths of intervals, becomes a poison random variable.

$$p(a, t) = \frac{1}{2a} \int u(x, t) dx$$

He went on to talk about the *Geometry of the System*.<sup>2</sup>Real surfaces have domains which have domain boundaries and step edges which form a bounded regions on the surface. Preferential growth takes place at these boundaries at a very high rate.

Next, the *Linear Model*, where reaction diffusion happens in the presence of reaction centres, which are located at radii  $r_1, r_2, \dots, r_N$ . There's a single at the boundary  $r = R$ . Particle flux is perpendicular to surface. We have some formulations here that has been skipped.

Reaction diffusion equations in the Laplace domain are written and then we can write the Green's Function for it. The solution is a linear set of equations, an  $N \times N$  matrix. He discussed in particular the ring model, and the point model

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<sup>2</sup>At this point I hope it's clear that I couldn't follow most of what I noted. Only people familiar with the topic have the remote possibility of gaining something from this. This seems useful other than that, only for evaluation purposes, although what it is supposed to be evaluating, is beyond my comprehension at this stage.



(point defects). He showed a simulation and its context remarked that the wall like structure exists since  $k_r$  is very large.

He then talked about *Stochastic Simulations Algorithm* based Smoluchowski equation, which went something like this

- (1) Drop a particle of type S at a random  $r$ , uniform in  $\sigma$
- (2) Choose a particle from the surface
- (3) Compute  $r_{i,t+\delta t}$  (there was a formula, which couldn't be noted)
- (4) Generate a random number  $\rho$ .  $\rho < k_i\delta t$  and  $r_{i,t+\delta t} \in \omega_j \forall 1 < j < N$ , perform the reaction step.
- (5) Goto 1

Then there are some results

- Mean first passage time

$$\langle t_f \rangle \sim \frac{C_1}{k_b + C_2}$$

where  $C_1$  and  $C_2$  are constants (positive) dependent on  $D_p$  (which was defined in an earlier part, which couldn't be noted)

- First passage time probability density

$$p(t_f) = A^2 t_f e^{-At_f}$$

He supplemented this with various diagrams and then moved on to describe a particularly simple example. Suppose we start with a constant concentration and after some time this is what it looks like, there'll be formation of clusters at the origin and decay of particles. If you were to take the gradient and analyse further, you'll find that more the number of atoms that come there (the clusters he meant) for the atoms, there's a repulsion which reduces the incoming rate.<sup>3</sup>

Towards the end, I could only list the topic titles he covered, which go from *Derivation from the master equation*, *Linearized Equations* to *Drift Diffusion Equations* and *Trapping reaction with self exclusion*. About the last topic, he said you could simulate for trapping with exclusion and numerically take the slope, however that is not a very simple test as the slope deals with a log term.

In conclusion, his second last slide (last being thank you) read

- (1) Presented a minimal model for cluster formation at nano-scales in the presence of surface defects
- (2) The linear model agrees qualitatively with the experiments
- (3) Effects of exclusion and non-linearity were studied

In the question answer session, there was a discussion on the exponent power  $\frac{1}{3}$  which is manifested if you wait for long enough in a constant rate reaction, say  $e^{-kT}$ , then it becomes  $e^{-\alpha kT}$ ; and this had been predicted earlier. Certain theoretical parts were clarified to not have been experimentally verified. Further, it was further clarified that no major work on quantum formulation of the same has been done. Most approaches were classical.

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<sup>3</sup>Again, I'm very sorry, I myself am lost and not certain in what context this is to be placed.

## CHAPTER 3

# Coherences, Photosynthesis and Quantum Biology

### 3.1. The Facts

**When, where and who.** The seminar was held on November 6, 2013, 3:00 PM, in LH 3 (LHC). The speaker was Prof. K. L. Sebastian (Department of Inorganic and Physical Chemistry, Indian Institute of Science).

**The Abstract.** It was believed that energy transfer within the photo-system involved exciton hopping from one site to the next. 2D electronic spectroscopic experiments carried out by Fleming et al., needed a modification of this view. The experiments suggested that at least in organisms living in extreme conditions, there is a wave like energy transfer and that evolution has optimized the process using quantum coherence. Since then the energy flow has been studied a lot, both theoretically and experimentally. Also it has been suggested that quantum mechanics is important in the most important biological process happening on earth, leading to the genesis of (according to some scientists) the subject of quantum biology. An overview of these studies and our theoretical work in the area will be presented.

### 3.2. What I could partially follow

Prof. Sebastian started with talking about claims about biological systems that perform quantum computation. The outline of the talk has been listed:<sup>1</sup>

- (1) Problem
- (2) Coherences
- (3) Environment - De-coherence
- (4) The FMO photo system
- (5) Coherences Experimental Observations
- (6) The Hamiltonian
- (7) Approach based on Adiabatic Basis
- (8) De-coherence and Population Relaxation
- (9) Summary

So let us start with the problem itself. The FMO complex (named after Scientists Fenna-Matthews-Olson, working in the field) consists of three chlorophyll monomers. Chlorophyll itself has 7 centres. You excite one of them, and the excitation can travel. There's one centre that transfers the energy to the reaction centre (number 3). The most prone to excitation however are two centres remote from number 3, namely number 1 and 7. This was clear from the diagram which hasn't been included here. It was earlier an accepted view that these excitations can jump from one to the next level, traditionally 'hopping'. However, more recent

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<sup>1</sup>This seminar has parts I could follow but couldn't deduce from prior steps. Thus this is only useful as proof of attendance, or at best to get an idea of the content of the talk.

experimental evidence seems to suggest that there exists a wave like mechanism as opposed to the popular Forster resonance mechanism. The experimental paper by Fleming et al (2007) showed that for such a picture, coherences are very important.

The speaker then went on to give a short introduction to coherence. He began by discussing a superposition state of two wave functions.

$$\psi = \psi_1 + \psi_2$$

The non-square terms in the square of  $\psi$  will constitute what is called coherence. For clarity, he asked us to imagine superposition of two electronic states, specifically the s and p states. The question then is what happens if we let this wave function evolve with time. We simply operate it with the time evolution operator in the position basis. When the square of this time evolved state is calculated, it turns out that the square terms are time independent but the coherent term picks up time dependence. This results in the oscillation of the wave function with time. He even showed a simple animation to get the point through.

The next important question was then how the environment effects the system. For a physical picture, one can imagine an electron surrounded by water. One way to proceed would be to start with considering the effect of the fields produced by the S orbital and P orbital separately. For the S orbital obviously the field would be radially symmetric. However for the P orbital it won't be. The environment (the water molecules) will be affected by this. The water molecules can be approximated as dipoles being acted upon by the field and they will re-orient, changing the environment itself, in response to the electronic field. This interference of the environment must be accounted for in the wave function of our system and as it turns out, this causes what is termed as 'decoherence'.

The speaker insisted on noting the distinction between relaxation and decoherence. This may be expressed mathematically as

$$\left(\frac{t_D}{t_g}\right)^2 = \frac{6k_bT}{\lambda}$$

where  $\lambda$  is the stokes shift and the other terms have obvious association.

The speaker then talked about an experiment in which 2D electronic spectroscopy was used to observe an interesting result. The speaker first described the result and then explained quickly how the experiment was performed. The result essentially was the visibility of oscillations of peaks in a biological system, as was expected from the aforesaid theory, lasting for about 600 fs. Typically they are expected to die out within 60 fs or so. There have been claims of oscillations lasting for over 1.2 to 1.5 ps also.

The explanation of the experiment was rather simplistic and not too deep. The idea was an application of a pulse sequence, which consisted of three pulses, each of 35 fs duration. The first pulse puts the ground state into a linear combination of ground and excited state. The second converts it to a predominantly excited state and the final pulse gets them back to the ground and excited state. The time between the first and second & the second and third can be changed experimentally. Thus the signal we get is a function  $S(\tau, T, t)$  which is Fourier transformed to the frequency domain  $S(\omega_0, T, \omega_1)$ . In the 2d spectrum then, with change in T, you can see the cross peaks and their amplitude oscillating.

Prof. Sebastian then went on to talk about the photo-system. This essentially consists of one monomer of the FMO complex. The energy difference between the Highest Occupied Molecular Orbital and the Lowest Unoccupied Molecular Orbital was stated to be about  $12,000\text{ cm}^{-1}$ . If we now look at the energy levels of each of these, then it is found that the one corresponding to centre number 3 (described earlier) is the least, as expected. The surroundings are essentially tuned so that the flow is towards the reaction centre. One can construct a Hamiltonian which as it turns out, goes as distance power minus three. This may be understood as some sort of dipole interaction for in two dipole interactions, we get the form  $1/R^3$ .

Prof. Sebastian then talked about donor and acceptor molecules. Suppose there are four orbitals, one ground and its corresponding excited and similarly another set. Now suppose a molecule gets excited from the lower to higher level. When this molecule comes back to the ground state, it interacts with the adjacent molecule and puts it in the excited state.

So the question now is how to describe such a system including the surroundings. Imagine now that you have 7 molecules. I take their Hamiltonian without worrying about the surroundings. I can consider the surroundings to be phonon like sites, with a Hamiltonian approximated by that of a harmonic oscillator. For each site I can write this. The coupling then will essentially cause fluctuations which results in the energy gaps going up and down, which as diagrammatically shown by Prof. Sebastian. Thus one can write the coupling as

$$H_{\text{el-ph}} = \sum Q_j |j\rangle \langle j|$$

So to solve the problem, the initial conditions are taken to be the exciton being at the  $j^{\text{th}}$  centre and the temperature bath at  $T$ . The Hamiltonian for this system however has one problem. The de-coherence and population relaxation are caused by the same term. There are no small parameters to do perturbation.

An alternative method is to numerically integrate, which a research group did in fact do. The other method is just as complex.

However, Prof. Sebastian's group took yet another approach and started with what is popularly known as the Born Openheimer approximation. For a fixed position, a hamiltonian is written and then the kinetic energy of the oscillators is added. The eigenfunction then for the Hamiltonian will correspond to the 7 centres. Reaching the solution to the Hamiltonian he explained wasn't straight forward for some terms do not commute. However, the final result is that moving energy levels are obtained. The method used involved a Markovian Master Equation.

The final result of all the hard work, was displayed on a very interesting slide. This had results from two different papers, numerically calculated points, on a population vs time (in femto seconds), together with Prof. Sebastian's curve, in complete agreement, for various centres of chlorophyll.

The speaker then went on to talk about how transfer between the eigenstates of the Hamiltonian considered had been ignored. If the surrounding's not ignored, then the oscillation doesn't last for long enough. Which is to say that without the population relaxation, the surroundings kill the oscillations very quickly. However, with population relaxation, you can see a transfer to site 3.

Some of the lurking questions were essentially to do with why the oscillations lasted for so very long and as it turns out, we can answer it in at least the following ways.

- (1) Protected by the protein
- (2) Not many water molecules
- (3) Change in dipole moment is small

Experimentally however, it has been found that there are various water molecules and they even change orientation which is enough to disturb the Hamiltonian. So in more realistic calculations, oscillations can't be observed.

The speaker concluded by stating that an almost analytic approach to the coherence problem was explored and presented. He also made use of adiabatic basis with decoherence and relaxation separated. And of course, the excellent agreement with the results.

The final remark was an answer to the question 'Are Bacteria Quantum Computing?'. According to the speaker, such quantum phenomena in biology, in his opinion, he doubts exist.

## CHAPTER 4

# Mechanics of Information Processing and Computation in Cells

### 4.1. The Facts

**When, where and who.** The colloquium was held on November 6, 2013, at 4:00 PM, in LH 3 (LHC). The speaker was Prof. Madan Rao (RRI, NCBS).

**The Abstract.** The surface of living cells reads and processes information from the ‘outside’ and transmits it to the ‘inside’. It does this by regulating the dynamics and organization of a variety of signalling molecules. We have shown how the dynamics and organization of many cell surface molecules can only be understood by its intimate coupling to an active cytoskeletal layer juxtaposed to it. We argue that the physical principles underlying the Active Composite cell surface provide the natural language for discussing the mechanics of computation and information processing at the cell surface. In connecting active mechanics in cells with information processing and computation, we bring together two seminal works of A. Turing.

### 4.2. What I could follow

The speaker opened with an amusing statement ‘I don’t need to complete the talk.’ encouraging questions and interaction from the very start. Dr. Rao initiated the content by stating how cells perform/compute, by molecules that exist within the cells, which requires the mechanics to be constructed by the cells in itself. So the basic unit, the cell is in the spot light. It has the basic characteristics of ‘life’. More specifically, Dr. Rao looked at the cell periphery in this talk in more detail, called the cell membrane. It is composed of thousands of kinds of lipids and other molecules.

On the surface of the cell, there exist various kinds of proteins which allow the cell to actively regulate the profile of the cell surface, via the cortical actin. This essentially is to say that the surface profile is governed by the *stuff* inside, not on the surface. Why the cells require energy for this can be understood by considering the following.

- (1) Cells regulate the organized collection of biomolecules  
(you need energy to beat the second law of thermodynamics; which is to say that to produce order, you need to expend energy)
- (2) The information is encoded in molecules or organization of molecules  
(Cells therefore regulate the organization of information; this too requires energy)
- (3) Organization-transport-transformation of molecules is the storage-flow-processing of information

The speaker then digressed to discuss a seminal work of AM Turing. In his work, Turing discussed mathematical explanations of various patterns observed in Biology. His 1952 paper<sup>1</sup> was based on the following minimalistic assumptions

- (1) The changes of position and velocity are as given by Newton's Law of Motion
- (2) The stresses are as given by the elastic motion, also taking into account the osmotic pressure as given from the chemical data  
(this however, for lack of biological interpretation, was not considered further)
- (3) The chemical reaction/rate laws
- (4) The diffusion of chemical substances; the region in which this diffusion is possible is given from mechanical data.

Prof. Rao then graphically demonstrated how using rather simple systems, one can obtain banded structures with length scales of  $\lambda = \sqrt{\frac{D}{k}}$ , where  $D$  is the diffusion rate and  $k$  is the degradation rate. The equations have been omitted for brevity. The speaker however stressed on the fact that the cell has been treated as a passive entity, as the forces and stresses had been ignored. He went on to state that the cellular medium is interactive; driven out of equilibrium. By moving the meshwork (the cytoskeletal filaments) one can shift the system off of equilibrium. And this process happens continuously, using various different kinds of molecular machines.

To understand the physics of stresses generated by the angular mechanics, Prof. Rao claimed we need a new kind of statistical mechanics, which is called *Active Cellular Statistical Mechanics*. It consumes energy and moves the cytoskeleton; Consume Chemical Energy (ATP)  $\rightarrow$  Cyclical Conformation Change  $\rightarrow$  Movement. This has consequences in patterning, fluctuations and mechanics of cells.

The next slide titled 'Treadmilling' was rather fascinating cause of its video content; this was the work of E Sheldon. The cartoon version of the experiment had projections on a planar surface which would move in specific patterns causing the overlying filaments to zoom past. This is precisely what was also observed experimentally. The movement speed was roughly  $0.4 \mu\text{m/s}$ .

It is important to note that the active forces in this context are internal forces, so then the net force is zero. The detailed analysis was skimmed through by the speaker, but the important relations mentioned were as follows.

- Active Current  $J\alpha n$ , polar orientation
- Active Stress  $S\alpha Q = nm$ , orientation tensor

Dr. Rao post this, looked at the percussions of applying active mechanics to the cell surface. As history has it, a 2D swimming pool model of lipid bilayer was widely accepted, more formally known as the picture of Fluid Mosaic (1972). This picture was challenged by new experimental evidence which showed a distribution of rafts associated protein richness. The number of each cluster is found to be around 4-5 maximum and their distribution is not the same as that in equilibrium. It was then found that the cell membrane is an active composite membrane, which is an open non-equilibrium system; driven by the activity of cortical actin meshwork, and not passive.

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<sup>1</sup>which was written at a time when there were no explanations for biological forces (motor proteins)

There are long static actin and small dynamic actin filaments. It is the interplay between them that gives rise to nano-clusters. The corresponding length scale  $\lambda$  (as stated earlier) which rises from the active current and active stress. Skipping the formal derivation, the equations yield asters (inward pointing) which form and break due to stochasticity. The strength of the aster as a function of time and of Local aster density vs Time (which was of the order of 0.1 to 1 seconds) graphs were shown. He also showed some results regarding the same using optimization simulations. This can be easily viewed as having a fixed number of sensors, trying to capture an image which is changing with the time. The problem then is, what is the best strategy (position of each sensor as a function of time) for getting the least error. Various graphs related to this were shown with the conclusion that it is better to form dynamic clusters when the density of sensors is low, and form a fixed lattice, when the number is high enough.

Next, 3 classes of cell membrane molecules were laid out.

- (1) Inert  
Doesn't interact with the dynamic actin
- (2) Passive  
Interacts with dynamic actin, but doesn't remodel it
- (3) Active  
Interacts with dynamic actin and remodels it

Now interestingly enough, in an in vitro design of a minimal cortical action system, different components, viz. Actin, Myosin, Filament and ATP were appropriately added and after the required labeling, one is able to see the formation of asters; This was demonstrated by a video of the actual experiment. As an experimental remark, Prof. Rao said that it is better to have a 3D system so that the removal of substrates is facilitated, as compared to restriction between glass slides.<sup>2</sup>

Now the question of computing comes. Given the three classes of cell surfaces plus asters (quasi-enzyme), one can create functions, which can be composed to make gates. That said, using Turing's model, one can perform all kinds of computations. However there are always energy consideration and optimal rates. The concept of mutual information (shannon) can be used to improve the accuracy. The possibility of chemical programming is thus manifested here. The condition however is that for regulatable information processing in finite time, the system needs to be driven out of equilibrium.

With that, the speaker ended the talk. Some questions which were interesting included one on the types of cells that have active cell membranes, and the answer to it was Eukaryotic Cells (specifically not bacterial cells). Another question was related to cryptography, which the speaker said is plausible exists for there are various instances where a cell must know the other cell's type. Further there are instances when cells try to imitate to be 'good guys' to penetrate. However, he claimed this hasn't been fully explored.

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<sup>2</sup>There were some more details which have skipped here, related to the aforesaid.