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Quantum tunnelling of the magnetisation in molecular nanomagnets

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The tunnel effect represents the fascinating point where quantum mechanics meets the classical world. Even though not very easily observable, quantum tunnelling in charge transport is a well known phenomenon, now even exploited in devices, as in the Super Conducting Quantum Interference Device (SQUID). On the contrary the tunnelling phenomenon in magnetic materials is much less investigated. Most of the properties that make magnetic materials so important in our every-day life, i.e. magnetic hysteresis and related memory effect, do not reveal any macroscopic quantum effect. However, if the dimensions of the magnetic material are shrunk below the width of a domain wall, all the magnetic moments move coherently and the process of magnetisation reversal occurs by the overcoming of an energy barrier originated by the magnetic anisotropy of the material.

This barrier can be crossed through a thermally activated process, but the presence of transverse anisotropy, or the application of a transverse field, can induce an underbarrier mechanism. The smaller the effective mass, here the magnetic moment that has to tunnel, the larger is the tunnel probability. Thus nanosized magnetic particles, comprising hundreds or thousands of coupled spins, are good candidate to show quantum tunnelling of the magnetisation (QTM), and even better are antiferromagnetic particles, where the magnetic moment is reduced to the uncompensated fraction on the surface.

In the eighties the theory of QTM experienced a fast progression, however the experimental evidences of QTM were rather blurred. The major problem is in fact due to the strong dependence of tunnelling on the axial and transverse magnetic anisotropy that, on their turn, are related to the dimensions of the nanoparticle. Ensembles of nanoparticles are unfortunately characterised by a distribution in size and shape.

**Molecular nanomagnets**

In the beginning of the nineties chemists, and in particular molecular chemists, entered into the game by starting to synthesize and investigate objects that can be seen as the “missing link” between the quantum word of paramagnetic metal centres and the classical one of magnetic particles. These new materials, known as molecular nanomagnets or as Single Molecule Magnets, are indeed clusters comprising a relatively small number of paramagnetic centres. These are usually paramagnetic transition metal ions, which interacts through bridging atoms, e.g. oxygen, or groups of atoms, e.g. the cyanide bridge. One example of this kind of molecules is the octanuclear iron cluster of formula [Fe₈O₂(OH)₆(tacn)₆]Br₆, abbreviated from here on as Fe₈, whose structure is shown in Figure 1. The coordination sites of the iron atoms are saturated by the organic ligand tacn=triazacyclonane, which provides a hydrophobic shell preventing the growth of the metal hydroxide-oxide core to an extended lattice.

The major advantage of the molecular approach, compared to the coating of nanosized particles, is that the clusters are arranged in a crystal structure and, in the most favourable cases neglecting also crystal defects, all the clusters are identical, equally oriented and weakly interacting among themselves. Despite the fact that oxygen atoms very often mediate moderate antiferromagnetic interactions, the complex connectivity and the related spin topology leads in some cases to a large spin multiplicity of the ground state. The example of Figure 1, Fe₈, possess a ground S=10 spin state. In this case the individual spins are those of rather isotropic, d⁵, iron(III) ions, with no orbital contribution. Also in the case of more anisotropic metal ions, as manganese(III), the orbital contribution is quenched by the low symmetry. Its presence is however important in the magneto-crystalline anisotropy, which is commonly described using an effective spin Hamiltonian of the form:

\[ H = D S_x^2 + E (S_x^2 - S_y^2) + g_\mu_B S \cdot H \]  

The first term is the axial anisotropy responsible for the energy barrier which separates “spin up” and “spin down” configurations as shown in Figure 2, where the states are labelled with the eigenvalue of S_z, M. The double well potential drawn in the figure is reminiscent of that observed in classical single domain particles. Here only 21 well defined levels are present but at low temperature the thermally activated reversal of the magnetisation follows an Arrhenius law and the characteristic time becomes macroscopically long. If it grows over the time needed to measure an hysteresis cycle, a remanent magnetisation appears, with a coercive field which increases on lowering the temperature. The
**FEATURES**

...hysteresis is not related to a cooperative phenomenon but is a property of the isolated cluster that behaves like a magnet, a Single Molecule Magnet. [1] In Figure 3 is reported the hysteresis loop of Mn12-acetate, the archetype of SMM, also characterised by S=10, whose well-known structure is also schematised in Figure 3. A large temperature dependent remanent magnetisation is observed and also almost equally spaced steps. This step-like hysteresis, discovered by the group of M. Sarachick in New York [2] and almost at the same time in Grenoble by the group of B. Barbara in collaboration with the group of D. Gatteschi in Florence, [3] is now considered the fingerprint of the tunnelling of the magnetisation and the reason is immediately clear by looking at Figure 2. The transverse terms in the spin Hamiltonian do not commute with the axial term at the origin of the barrier and admix the left and right well localised states, thus allowing an under-barrier mechanism. The extent of this delocalisation is larger in the states close to the top of the barrier and maximum when the unperturbed levels on the opposite sites of the barrier are degenerate. In zero field (see Figure 2) all the pairs coincide in energy and this corresponds to the most favourable condition to observe tunnelling. Depending on the temperature and the thermal population of the levels, tunnelling between the ground states or levels higher in the barrier can compete with the thermally activated mechanism, and a short-cut of the barrier occurs with a significant acceleration of the magnetic relaxation. When a longitudinal field is applied the ±M pairs are not in coincidence any more and tunnelling is suppressed, as in Figure 2b, except for critical values of $H_z$ for which the levels are brought in resonance again. According to equation (1) pairs of level are in resonance for $H_z = nD/g\mu_B$, with n integer, as clearly seen in Figure 4. Accelerations of the relaxation due to tunnelling occur at these fields, which correspond to the steps in the hysteresis curve. This mechanism was indeed first proposed by M. A. Novak and this author at the conference on “Macroscopic Quantum Tunneling of the Magnetization” held in 1994 close to Grenoble, where for the first time chemists introduced these novel materials to the physics community. [4]

Going back to Figure 2, a transverse field can be the source of the tunnelling, but when at low temperature pure tunnelling between the ground doublet occurs, a trivial calculation shows that a moderate field is not efficient enough, as it acts at the (2S)th order of perturbation only. A transverse anisotropy is however always present, of second order in the absence of any symmetry as in (1), or of higher order, depending on the symmetry manifold of the molecule.

**Topological interference**

Intuitively one would expect that the application of a transverse field would anyhow enhance the tunnel process, but this is not the case. By exploiting arrays of micro SQUIDs it has been possible to monitor the reversal of the magnetisation by sweeping the longitudinal field back and forth on a tunnel resonance, which is actually an avoided level-crossing between two levels, as shown in Figure 4. The probability of reversing the magnetic moment depends on the sweeping rate and on the tunnel splitting $\Delta$, i.e. the gap at the avoided level-crossing, according to the Landau-Zener-Stückelberg formula:

$$P_{M,M'} = 1 - \exp\left(\frac{-\pi\Delta^2_{M,M'}^2}{2h\mu_B |M-M'| \mu_O \frac{dH}{dt}}\right)$$

where $dH/dt$ is the field sweeping rate. The tunnel splitting $\Delta$ is then extracted from (2) knowing P by the fraction of molecules that has reversed magnetisation. The measurements performed on Fe8 in the pure tunnelling regime at very low temperature, with the procedure repeated for increasing transverse static fields applied along the axis of hard magnetisation, have shown the results reported in Figure 5. If the axial field is swept back and forth around zero then the tunnelling splitting investigated is the one between the ground M=±10 states. In this case the tunnelling is larger for zero transverse field, decreases to a very small value ca. 0.2 T showing an almost complete quenching, and then increases again. An oscillatory behaviour is seen with an almost
constant period in the whole investigated region. [5] On the contrary, if the transverse field is applied along the intermediate axis of magnetisation, the tunnel splitting increases steadily. The oscillatory behaviour has the semi-classical physical description that is schematised in Figure 6. The sphere represents the continuum of orientation that a semi-classical spin can assume; Z corresponds to the easy axis of magnetisation, while X and Y are the hard and intermediate ones, respectively. Let's assume that a static transverse field is applied along X. The system can be prepared in such a way that S is pointing toward A by applying also a magnetic field along +Z. Then the longitudinal field is removed and the two orientation A and B becomes equally probable. An ensemble of molecules will show initially a net magnetisation pointing toward +Z but at the equilibrium half of the molecules must be pointing their spin toward B. As the X direction is the less favourite one the spin will tend to rotate in a plane which is parallel to the YZ plane. The tunnelling transition from A to B on the sphere of Figure 6 can therefore occur along two equivalent paths, one clockwise and the other anti-clockwise. The two paths can interfere destructively leading to the quenching of the tunnel splitting experimentally observed. The topological nature of the interference, even if in the spin space, has suggested for this phenomenon the name of magnetic Berry phase effect. The destructive interference occurs when the area highlighted in Figure 6 is equal to kπ/5, with k an odd integer. This argument was presented by A. Garg some years before its experimental realisation, [6] when a large but well defined spin was still considered a text-book assumption. If we limit our analysis to the second order transverse anisotropy reported in (1) the quenching occurs when the transverse field assumes the values:

\[ H_x = \frac{2n+1}{g\mu_B} \sqrt{E(E+D)} \]  

(3)

where \( n \) is an integer. It is important to stress that at these fields an exact degeneration not related to the Kramers theorem occurs and this is an exception to the general rule that "levels repel each other". This situation is so exceptional that is sometime described as "diabolic". In this case the number of observed "diabolic fields" with quenching of the tunnel splitting is 10 on each field sign. This number corresponds also to how many times the perturbation induced by the E term in (3) must be applied to connect the two states involving the tunnelling. A numerical diagonalisation of the spin-Hamiltonian matrix allows one also to take into account different orientations of the transverse field in the XY plane. However one can immediately visualise that, when the transverse field is applied along the Y direction, one tunnel pathway is favourable and no destructive interference is possible, as indeed is experimentally observed.

If the experiment is repeated by sweeping the longitudinal field around a value which corresponds for instance to the \( M=10 \rightarrow M'=-9 \) resonance, thus \( H_2=g_2\mu_B \), the transverse field dependence of the oscillation is completely different, as shown in Figure 5. Where maxima in tunnel splitting were previously present, minima are now observed, and vice versa. Now the two states are connected by an odd number of steps, exactly as in the case of half-integer spin states. The parity effect related to the time-reversal suggests that the tunneling must be quenched in zero transverse field as experimentally observed. When the field is swept around \( H_2=g_2\mu_B \), bringing \( M=10 \) and \( M'=-8 \) in coincidence the oscillations have the same phase as for the \( M=10 \rightarrow M'=-10 \), as shown in Figure 5. By simply changing the value of the field it is possible to modify the parity of the system.

All these experiments have provided elegant evidences of the tunnel mechanism in nanomagnets, and for these results the principal investigators (B. Barbara, J. Friedman, D. Gatteschi, W. Wernsdorfer and this author) have been awarded with the 2002 Agilent Technologies Europhysics Prize. Many other scientists have contributed to shed light on this new phenomenon by performing experiments that range from neutron spectroscopy to magnetic resonance, from muon spectroscopy to specific-heat measurements. Parallel to the experimental work, the contributions of many theoreticians have turned this field to what J. Villain has called "a school of physics".

**The role of the environment**

The story is however more complex than how it has been depicted up to now. In fact, it is sufficient to note the order of magnitude of the tunnel splitting in Figure 5 to immediately realise that some other mechanisms must be active to promote tunnelling. A tunnel splitting in the ground \( M=\pm 10 \) doublet of the order of \( 10^{-7} \) K requires that any bias field is smaller than \( 10^{-8} \) T. Otherwise the level degeneracy, within the tunnel splitting, is removed and the admixing of the states is suppressed. Such a narrow tunnelling resonance could hardly be observed and indeed the experiments reveal tunnelling resonances, which are order of magnitude broader than this value. The clusters are not isolated objects but experience the dipolar field of the surrounding clusters in the crystal and a distribution of internal field is therefore expected. The origin of this field is the magnetisation of the molecules themselves, which is completely frozen at very low temperature if tunnelling does not occur. With a distribution width of the order of \( 2\times 10^{-2} \) T and an intrinsic width of \( 10^{-4} \) T tunnelling should be a very rare event, unless the external field is swept over the entire distribution, as is the case for the Landau-Zener-Stückelberg type of experiment.

Prokof'ev and Stamp have proposed that at very low temperature tunnelling between the \( \pm S \) pair can only occur if the fluctuating nuclear magnetic field is taken into account. [7] This fluctuating field has the effect of bringing in resonance the couple of levels where tunnelling is expected to occur. The reversal of the magnetic moment of a molecule inside the crystal modifies the dipolar field of the neighbouring sites and other molecules are...
thus brought close to the resonance condition where the fluctuating hyperfine field can be efficient again in promoting tunnelling. A pictorial representation of the phenomenon could be a box of small spheres and a small hole. If everything is static only the sphere that accidentally is over the hole can exit the box. However, if the box is gently shaken, the hyperfine field, more spheres among the ones close to the hole, have the chance to go through it. As soon as a sphere exits the box the hole moves to a different region of the box and here the process restart. The theory developed by Prokof'ev and Stamp predicts that at short times the relaxation shows a square root time dependence of the decay of the remnant magnetisation, that has been indeed experimentally observed and also reproduced by using Monte Carlo simulations. Transverse internal fields, of dipolar or nuclear origin, are also responsible for symmetry forbidden transitions.

The distribution of tunnel splitting can be investigated experimentally by using a technique, which is well known in single molecule spectroscopy: the hole digging. The results of these experiments have revealed that at high temperature the line has a lorentzian shape and no holes can be dug. The linewidth is dominated by the homogeneous broadening induced by the larger tunnel splitting between levels, which are higher in the barrier. On the contrary at very low temperature a hole can be burnt and the intrinsic width of the hole is strongly dependent on the hyperfine field generated by the nuclei. This has been shown by measuring also two isotopically modified samples of the Fe8 molecular nanomagnets. In particular the substitution of the non-magnetic 56Fe nuclei with 57Fe possessing I=1/2 increases the hyperfine field, which, on the contrary, can be reduced by replacing hydrogen with deuterium. Unfortunately the large contribution due to the nuclei of 16O in the tacn ligand cannot be modified. Anyhow a significant increase in the linewidth of the hole dug in the tunnelling resonance is observed. The 57Fe isotope has the largest linewidth and the fastest relaxation and the deuterated sample shows the narrowest resonance and the slowest relaxation.

The role of nuclear magnetism is even more important in another class of materials of different origin but with many analogies with molecular nanomagnets. B. Barbara and co-workers have shown that rare earth anisotropic ions, like Ho3+, in the diamagnetic host lattice, LiYF4, can experience an energy barrier which hampers the magnetisation reversal. The interaction of the electronic ground doublet with the 1=7/2 nuclear magnetic moment of the Ho3+ ions gives rise to a stepped hysteresis where the steps correspond to avoided level crossings within the 16 manifold of the hyperfine splitted doublet.

The detailed investigation of the dynamics of the magnetisation of molecular nanomagnets has also revealed other important effects. Recently W. Wernsdorfer, in collaboration with American chemists G. Christou and D. N. Hendrickson, has investigated a wide range of tetranuclear manganese clusters and in one of them the clusters are coupled in pairs by hydrogen-bonds. The effects of these interactions on the tunnelling are well evident. The quantum transition in zero longitudinal field, which corresponds to the simultaneous tunnelling of both spins of the pair, is suppressed and other transitions are observed that are assigned to spin cross-relaxation.[8]

Crystal defects or disorder effects in Mn12-acetate leading to deviations from the tetragonal symmetry have also been the subjects of recent theoretical and experimental studies. This could appear as a contradiction, suggesting that the systems are not so ideal as initially proposed. On the contrary only "clean" systems and "clean" experimental results can allow an investigation of the nature of the defects by looking at their effects on the quantum dynamics of the magnetisation.

Possible applications
Up to now we have attended "the school of physics" provided by these elegant applications of quantum mechanics but the Agilent Technologies Europhysics Prize awards fundamental works "leading to advances in the fields of electronic, electrical and materials engineering". How can our research fulfill these expectations? It is trivial to say that in the materials we have investigated each molecule behaves as a magnetic memory unit, but it is hard to conceive a PC hard disk made of Mn12-acetate. First of all we have to learn how to address a single molecule. We have seen that the effects of the environment are far from negligible and to monitor them chemists are now going beyond the single crystal samples and are organising the molecules in a controlled way, for instance attaching them on the surface of a conductor. The topologic interference effect, if observed in other magnetic materials, could be exploited to achieve a better control of the magnetisation process, which is very important to obtain stable and easily writable mag-
magnetic supports. Leuenberger and Loss have also tried to visualise the exploitation of molecular nanomagnets for quantum computing [9] but an experiment based on their ideas has not yet been realised. We have first to learn to control the tunnelling process by using an electromagnetic field. Chudnovsky and Garanin have even proposed the existence of a super-radiance phenomenon if the tunnelling transition is swept rapidly enough to achieve the population inversion and all the spins tunnel in a coherent way. Some experiments have been recently performed, on Mn12-acetate crystals again.

The story is far from coming to an end, also because there is no limit to the ingenuity and fantasy of chemists. They continue in designing and "creating" novel molecules that range from one dimensional magnetic systems closed on themselves to provide magnetic rings of various size, to buckyball magnetic clusters that seem to have lost most of their quantum nature.

We have reached the end of this short overview where a chemist has been invited to write in a physical magazine. This fact reminds me of a dialogue between Primo Levi, a famous writer but also an enthusiastic chemist, and the Italian physicist Tullio Regge. I find the words of Regge "The universe must be infinite to realise everything is permitted, because what is permitted is also compelled to be" very adequate to describe the role that chemists have played in this story. Chemists have just condensed more of these possibilities in small molecules. We have then served to physicists these little toys to observe hidden phenomena of quantum mechanics that, after all, had to be observed.

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Crowd control
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The application of ideas, methods and results of statistical physics to a wide range of phenomena occurring outside of the realm of the non-living world has gained a great momentum recently. Among many others, examples include the studies of various group activities of people from the physicist's viewpoint. Here, I shall give a partial account of some of the new investigations in this direction, involving the interpretation of such collective human activities as group motion and synchronisation.

On the small scale side of the size/complexity spectrum, in the world of atoms and molecules collective behaviour is also considered to be an important aspect of the observed. Furthermore, there are articles on collectively migrating bacteria, insects or birds and additional interesting results are published on phenomena in which groups of various organisms or non-living objects synchronise their signals or motion. This is the natural scientist's aspect of how many objects behave together. However, if you search for a collective behaviour related item with your web browser most of the texts popping up will be concerned with group activities of humans including riots, fashion or panics.

What is common in these seemingly diverse phenomena involving interpretations ranging from social psychology to statistical physics? The answer is that they happen in systems consisting of many similar units interacting in a relatively well defined manner. These interactions can be simple (attraction/repulsion) or more complex (combinations of simple interactions) and may take place between neighbours in space or on a specific underlying network. Under some conditions, in such systems various kinds of transitions occur; during these transitions the objects (particles, organisms or even robots) adopt a pattern of behaviour which is nearly completely determined by the collective effects due to the presence of all of the other objects in the system.

Take ferromagnets as an example. These materials can undergo spontaneous magnetisation, in effect because they are made up of a host of "tiny magnets". At relatively high temperatures, these magnets cannot align with each other and the resulting magnetisation is zero. But at a critical temperature the tendency to adopt a common direction suddenly, but continuously takes over from the effects of fluctuations. So, most of the small magnets, assisting each other in a collective manner, point in the same direction, and magnetisation (order) spontaneously appears. Similarly, a group of feeding pigeons randomly oriented on the ground will order themselves into a uniform flock while flying away after a big disturbance.

Fig. 1: Spontaneous formation of lanes in a system of oppositely driven particles with repulsive interactions. Similar segregation of pedestrian flows can be observed, e.g., along wide corridors.
Motivation
Mankind has been experiencing a long successful period of technological development. This era has been the result of a deeper understanding of the various physical and chemical processes due to the outstanding advances in the related sciences. After these achievements there is now a growing interest in a better, more exact understanding of the mechanisms underlying the main processes in societies as well. There is a clear need for the kind of firm, reliable results produced by natural sciences in the context of the studies of human behaviour. The revolution in information and transportation technology brings together larger and larger masses of people (either physically or through electronic communication). New kinds of communities are formed, including, among many others, internet chat groups or huge crowds showing up at various performances, transportation terminals or demonstrations. Since they represent relatively simple examples, these groups or communities of people provide a good subject from the point of studying the mechanisms determining the phenomena taking place in societies.

In the following I would like to show that the concept of collective phenomena can be applied to the group behaviour of people. In a way understanding a new phenomenon is usually realised by relating it to a known one; a more complex system is understood through analysing its simpler variants. In the seventies there was a major breakthrough in statistical physics when a deep theoretical understanding of a general type of phase transitions was achieved due to the invention of the so called renormalisation group method. This theory showed that the main features of transitions are insensitive to the details of the interaction between the objects in a system, thus, as an extreme case, orientational forces between atoms may result in ordering phenomena similar to those observed in groups of much more complex units.

Below we discuss new quantitative approaches to collective behaviour based on the exact methods of statistical physics. It is clear that the methods developed in natural sciences contain a significantly smaller amount of subjectivity than those used for the interpretation of human behaviour. If more exact approaches could be applied to social situations they could provide the desired objectivity, reproducibility and predictability. We demonstrate that in cases when the interactions between the members of a group are relatively well defined (e.g. pedestrian traffic, rhythmic applause, panic, soccer fans in stadiums, etc) the corresponding numerical models reproduce relevant aspects of the observed phenomena. Simulating models in a computer has the following advantages: i) by changing the parameters different situations can easily be created ii) the results of an intervention can be predicted and iii) more efficient design of the conditions for the optimal outcome can be assisted. In addition to possible applications, our approach is useful in providing a deeper insight into the details of the mechanisms determining collective phenomena occurring in social groups. Most of the results I am discussing next are available through the home page given in Ref. [1]. There exist additional remarkable efforts in similar directions by groups working on traffic, evacuation dynamics, econophysics and on further related topics (see, e.g., Refs 2-4).

Methods
Our central statement is that collective behaviour can be very efficiently studied by the methods developed by statistical physicists. The related theoretical and numerical approaches provide reliable, sometimes exact description of the processes taking place in many particle systems. We assume that under some conditions a large group of humans can be considered as a collection of particles, since there are various situations where the interaction of people is reasonably well defined (e.g., two people heading towards each other in a corridor will avoid each other just as if they had a repulsive physical force acting between them). For the last two decades perhaps the most fruitful approach to the study of collective phenomena has been the application of computer simulations. In such studies a simple model is constructed which is supposed to grab the most relevant features of the system to be studied. Then, by letting the algorithm run in the computer while monitoring the parameters of the models a great variety of collective phenomena can be observed. The true test of a model is a careful comparison of its predictions with the behaviour of the real system.

Examples
The rest of the paper will present examples of group behaviour of people which could be successfully interpreted by computer simulations and the related theoretical concepts. It is hoped that the process of simultaneous investigation of particular examples and the abstraction of their most general features will in time lead to a coherent theoretical description of collective human behaviour.

Collective motion
Here we first address the more general question whether there are some global, perhaps universal features of collective motion [5]. Such behaviour takes place when many organisms are simultaneously moving and parameters like the level of perturbation or the mean distance between the individuals is changed.

1. One-dimensional case: Let us first consider a simple case of the particles (people) moving along a line (very narrow corridor, so that two people cannot get around each other). The particles are
trying to maintain the same speed except when they are forced to turn back. There are only two rules: a) Follow the others, or in other words, try to take on the average velocity of your neighbours (who all move left or right). b) In addition, an amount of randomness is added to the actual velocity (to account for example for the level of excitement of the pedestrians).

Simulations result in a completely disordered motion if the level of perturbations is large (each particle moves back and forth randomly). However, if the noise is smaller than a critical value (just as in the case of the ordering of ferromagnets), groups of particles are spontaneously formed the groups merge (aggregate) and sooner or later join into a single large group moving in a direction determined in a non-trivial way by the initial conditions. In the first, disordered case the people stay "trapped" in the corridor, even in the case of fire, while the ordered motion corresponds to a chance for escaping.

2. Two dimensions: Here the particles can get around each other and the pattern of motion is changed. Nevertheless, using the rules of "follow the others" and the application of perturbations leads to a transition from a disorderly moving crowd to an ordered "flock" when the level of perturbations is lowered.

A) Consider, as a thought experiment, thousands of people standing on a square and trying to look in the same—however, previously underdetermined—direction, after being asked to do so. A nice example for human collective behaviour would be if all of them managed to face the same direction. Can they do it? Statistical physicists can predict for sure that this cannot be done. They recall a theorem valid for particles with short ranged ferromagnetic interactions stating that in two dimensions no long range ordered phase (all magnets pointing in the same direction) can exist in such a system for any finite temperature and zero external field. So what happens? Locally people are looking almost in the same direction, but on a large scale, e.g., seen from a helicopter—just as the little magnets—they locally form vortex-like directional patterns due to the small perturbations due to human errors. Curiously enough, if the crowd is allowed to choose from a few discrete directions, the ordering can be realised. Perhaps even more interestingly, our models of flocking (based on the follow the neighbours rule) predict that if the people are asked to move in the same direction they will be able to do it.

B) In the latter models, if the moving particles are confined to move around in a closed circular area stable motion can be maintained only by the simultaneous rotation of all of the objects around the centre. Remarkably enough, under some conditions even humans move in groups in a manner predicted by simple models. Indeed, in Mecca each year thousands of people circle around the Kabah stone as they are trying to both keep on moving and not confronting with others.

C) Next we focus on a system of oppositely moving pedestrians in a corridor. Here the corridor is wide enough (its width is several times larger than the diameter of a person). Half of the pedestrians is assumed to move from left to right, the rest in the opposite direction. In the associated model it is assumed that the particles tend to take on a constant speed in their desired direction and are avoiding each other due to a repulsive force.

Simulations of this simple model based on the solution of the corresponding Newton's equations of motion reproduce the experimentally observed behaviour surprisingly well. A spontaneous formation of lanes of uniform walking directions in "crowds" of oppositely moving particles can be observed (Fig. 1). It is clear that lane formation will maximise the average velocity in the desired walking direction which is a measure of the "efficiency" or "success" of motion. Note, however, that lane formation is not a trivial effect of this model, but eventually arises only due to the smaller relative velocity and interaction rate that pedestrians with the same walking direction have. Once the pedestrians move in uniform lanes, they will have very rare and weak interactions.

Panics

One of the most disastrous forms of collective human behaviour is the kind of crowd stampede induced by panic, often leading to fatalities as people are crushed or trampled. Sometimes this behaviour is triggered in life-threatening situations such as fires in crowded buildings; at other times, stampedes can arise from the rush for seats or seemingly without causes. Although engineers are finding ways to alleviate the scale of such disasters, their frequency seems to be increasing due to greater mass events. Next we show that simulations based on a model of pedestrian behaviour can provide valuable insights into the mechanisms of and preconditions for panic and jamming by incoordination [6].

The available observations on escape panic have encouraged us to model this kind of collective phenomenon in the spirit of self-driven many-particle systems. We assume, in addition to the earlier considered socio-psychological forces the relevance of physical forces as well since the latter ones become very important in the case of a dense crowd with strong drive to get through a narrow exit. Each pedestrian of mass \( m \) likes to move with a certain desired speed \( v_l(t) \) into a certain direction \( e_l(t) \), and therefore tends to correspondingly adapt his or her actual velocity \( v(t) \) with a certain characteristic time \( \tau \). Simultaneously, he or she tries to keep a velocity-dependent distance to other pedestrians \( j \) and walls \( W \). This can be modelled by "interaction forces" \( f_{ij} \) and \( f_{iw} \), respectively. In mathematical terms, the change of velocity in time is then given by the acceleration equation

\[
\frac{m_i \, dv_i}{dt} = m_i \left( v_l(t) e_l(t) - v_i(t) \right) / \tau + \sum_j f_{ij} + f_{iw}
\]

The \( f_{ij} \) interaction forces include an exponentially decaying, repelling term expressing socio-psychological effects, and two additional "physical" terms corresponding to elastic repulsion and friction forces between the bodies of people.

The \( f_{iw} \) interaction with the walls is treated analogously. To avoid model artefacts (gridlocks by exactly balanced forces in symmetrical configurations), a small amount of irregularity of almost arbitrary kind is needed. This irregularity was introduced by uniformly distributed pedestrian diameters \( r \) in the interval \([0.5m, 0.7m]\), approximating the distribution of shoulder widths of soccer fans.
Based on the above model assumptions, it is possible to simulate several important phenomena of escape panic. The simulated outflow from a room is well-coordinated and regular, if the desired velocities are normal. However, for desired velocities above 1.5–m/s, i.e., for people in a rush, we find an irregular succession of arch-like blockings of the exit, a slow avalanche-like bunching of leaving pedestrians, when the arches break. "Faster-is-slower effect" due to impatience: Since clogging is connected with delays, trying to move faster can cause a smaller average speed of leaving, if the friction parameter is large (Fig. 2). This effect is particularly tragic in the presence of fires, where the fleeing people reduce their own chances of survival. Improved outflows can be reached by columns placed asymmetrically in front of the exits, preventing the build up of fatal pressures.

Finally, we investigate a situation in which pedestrians are trying to leave a smoky room, but first have to find one of the invisible exits. Each pedestrian may either select an individual direction or follow the average direction of his neighbours in a certain radius or try a mixture of both. We assume that both options are weighted with some parameter (1-p) and p, respectively, where 0<p<1. As a consequence, we have individualistic behaviour if p is low, but herding behaviour if p is high. Our model suggests that neither individualistic nor herding behaviour performs well. Pure individualistic behaviour implies that each pedestrian finds an exit only accidentally, while pure herding behaviour implies that the complete crowd is eventually moving into the same and probably blocked direction, so that available exits are not efficiently used, in agreement with observations. Accordingly, we find optimal chances of survival for a certain mixture of individualistic and herding behaviour, where individualism allows some people to detect the exits and herding guarantees that successful solutions are followed by the others (Fig. 3).

**Synchronisation**

1. Rhythmic applause: An audience expresses appreciation for a good performance by the style and nature of its applause. The initial thunder often turns into synchronised clapping—an event familiar to many who frequent concert halls. Synchronised clapping has a well defined scenario: the initial strong incoherent clapping is followed by a relatively sudden synchronisation process, after which everybody claps simultaneously and periodically. This synchronisation can disappear and reappear several times during the applause. The phenomenon is a delightful expression of social self-organisation, that provides a human scale example of the synchronisation processes observed in numerous systems in nature [7].

The above scenario can be recorded and the recordings analysed using the techniques common in physics [8]. The analysis reveals various interesting features including a spontaneous period doubling (as compared to the natural period of a single spectator) when the synchronisation takes place. In other words, after an initial asynchronous phase, characterised by high frequency clapping (Mode I), the individuals synchronise by eliminating every second beat, suddenly shifting to a clapping mode with double period (Mode II) where the dispersion (the relative difference in the clapping frequencies) is smaller. Statistical theories developed for a group of globally coupled periodically behaving objects can be used to demonstrate that the necessary condition for synchronisation is that dispersion has to be smaller than a critical value. Consequently, period doubling emerges as a condition of synchronisation, since it leads to slower clapping modes during which significantly smaller dispersion can be maintained. Thus, the evaluation of the measurements offers a key insight into the mechanism of synchronised clapping: fast clapping synchronisation is not possible due to the large dispersion in the clapping frequencies. After period doubling, as Mode II clapping with small dispersion appears, synchronisation can be and is achieved. However, as the audience gradually decreases the period to enhance the average noise intensity, it gradually slides back to the fast clapping mode with larger dispersion, destroying synchronisation (Fig. 4).

2. Mexican wave, becoming widely known during the 1986 World Cup held in Mexico, has since become a favourite paradigm for a variety of systems in which an initial perturbation propagates in the form of a single "planar" wave. The most important reason for the increasing popularity of this phrase, also known as La Ola, (or simply "the wave"), is likely to be due to its unique origin; it means a human wave moving along the stands of stadia as one section of spectators stands up, arms lifting, then sits as the next section does the same.

Using video recordings we have analysed 14 waves in stadiums with above 50,000 people: the wave has a typical velocity in the range of 12 m/s (20 seats/s), a width of about 6-12 m (~15 seats) and more frequently rolls in the clockwise direction [9]. It is generated by the simultaneous standing up of not more than a few dozens of people and subsequently expands over the entire tribune acquiring its stable, close to linear shape. (see page http://angel.elte.hu/wave) dedicated to this research, offering further data and interactive simulations).

The relative simplicity of the Mexican wave allows us to develop a quantitative treatment of this kind of collective behaviour by building and simulating models accurately reproducing and

**Fig. 4**: Fourier-gram of the clapping sound intensity after a great performance in one of the many theatres in Budapest. Grey level indicates the amplitude of the Fourier spectrum for the given frequency. Time is shown along the horizontal axis. The occurrence of the doubling and the subsequent decrease of the global period is indicated to happen several times.

**Fig. 5**: This figure shows the probability of generating a Mexican wave as a function of the number of the initiators and a parameter c corresponding to the critical level of excitement beyond which a person becomes active.
predicting the details of the associated human wave. It can be shown that the well established approaches to the theoretical interpretation of excitable media—originally created for describing such processes as forest fires or wave propagation in heart tissue—can readily be generalised to include human social behaviour. In analogy with models of excitable media, people are regarded as excitable units: they can be activated by an external stimulus (a distance and direction-wise weighted concentration of nearby active people exceeding a threshold value). Once activated, each unit follows the same set of internal rules to pass through the active (standing and waving) and refractory (passive) phases before returning to its original, resting (excitable) state.

Next, we employed these models to get an insight into the conditions for triggering a wave (Fig. 5). Our results clearly demonstrate that the dependence of the eventual occurrence of a wave on the number of initiators is a rather sharply changing function, i.e., triggering a Mexican wave requires a critical mass. This approach is expected to have implications for the treatment of situations where influencing the behaviour of a crowd is desirable. In particular, in the context of violent street incidents associated with demonstrations or sport events, it is essential to know under what conditions groups can get control over the crowd and how fast and in which form this perturbation/transition can spread.

Conclusions
The models of collective behaviour of humans can account for a number of specific features of social behaviour under certain conditions. The advantage of the models is that by changing the parameters different situations can be easily created. Models adequately describing group phenomena can be used for predictions. In addition to such more concrete possible applications of simulations as the design of escape routes or better networks, the models are useful in providing a deeper insight into the mechanisms behind such collective phenomena as synchronisation or panic.

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References
Controlling the flow of electromagnetic waves

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We shall not cease from exploration and the end of our exploring will be to arrive where we started and know the place for the first time.

T.S. Eliot

Waves in periodic media

The importance of waves in the natural and the man-made world can hardly be overestimated. We see and we hear through waves. We transmit information through waves. We understand and control the electrical, magnetic, and other properties of metals and semi-conductors through electronic waves. The latter propagate most often under the influence of a periodic (in space) potential due to the crystalline placement of the ions.

Waves in periodic media exhibit usually some common characteristics: The most important is the possibility of appearance of stop bands (also called gaps) separating pass bands (also called bands). This means that the frequency axis may be divided into alternating regions of gaps and bands: In the former, waves cannot propagate (cannot even exist in an infinite periodic medium), while in the latter they propagate freely due to constructive interference of the waves scattered by the periodic medium. The gaps appear as a result of destructive interference and/or the possible existence of non-accessible regions in space. Furthermore, a local deviation from the periodicity may trap the wave around it giving rise to an eigenfrequency in the gap. Attractive (i.e. negative) deviations tend to pull states out and below the bands, while repulsive ones (i.e. positive) tend to push states out and above the bands.

This picture allowed us to understand the distinction between conductors and insulators and formed the basis of the creation of solid state electronics.

The fact that electromagnetic (EM) and acoustic (AC) waves do not naturally propagate in periodic media and the focus on electronic waves in solids delayed until the late 80s the study of propagation of EM and AC waves in periodic media[1-4]. Actually this problem came to attention indirectly as a way of studying experimentally the localization problem in random media[4] or creating more efficient lasers[2]. Thus, through the helical path shown in Fig. 1 we arrived at the so called photonic band gap materials, or more simply photonic crystals[5-7], i.e. artificial periodic structures (with unit cell size ranging from about one micron to a few centimeters) exhibiting gaps (or pseudogaps) in the photon density of states (DOS) due to strong scattering and destructive interference; we arrived, so to say, where we started in the late 20s and early 30s.

A photon propagating in a photonic (PC) crystal is slowed down as its frequency approaches a gap, and finally its group velocity vanishes at the edge of a band as shown in Fig.2a. In other words, near the edge of a band, the behavior of a photon changes from that of a massless relativistic particle to that of a massive non-relativistic particle capable of being trapped around a local defect (see ref. 5, p. 86), like an electron in a doped semiconductor.

Furthermore, no photon can exist inside a large (theoretically infinite) photonic crystal for frequencies belonging to a gap. As a result, an atom or a molecule implanted in the interior of a large photonic crystal would remain in the first excited state, since spontaneous emission is inhibited, provided that the relevant excitation energy (divided by Planck’s constant) falls within the gap. The transmission coefficient of em waves of gap frequency exhibits a dramatic drop (see Fig.2b) providing thus a direct way to experimentally determine the gap.

Fig. 1: The helical time path leading from Bloch’s paper on electronic wave propagation in crystalline solids to photonic and phononic crystals.

Fig. 2: (a) Sketch of the dispersion curve, \( \omega = \nu k \), in a photonic crystal (solid line) and in the vacuum (dashed line). Near the gap the group velocity of the photon in the PC is reduced and the photon acquires an effective mass.
(b) Measured transmission coefficient of em waves vs frequency for the layer by layer structure[11] shown in Fig.4a; the corresponding dispersion curve is shown in Fig.3. At the gap the transmission is reduced by several orders of magnitude.
(c) The photon density of states (DOS) as calculated for a closed-packed fcc photonic crystal consisting of air spheres in silicon; notice the pseudogap at \( a/\lambda_c = \omega a/2\pi c = 0.52 \) and the gap around 0.8.
The photonic density of states (DOS) in a PC, in contrast to that of the free photon case, exhibits a complicated behavior with sharp peaks, abrupt dips, pseudogaps and true gaps as shown in Fig.2c. For low frequencies, i.e., wavelengths much larger than the lattice spacing, the PC appears to the wave as uniform and, consequently, the DOS is proportional to $\omega^2$ as in the free photon case. As the wavelength becomes comparable to the spatial periodicity, $a$, (and the sphere radius as well), the DOS exhibits strong variations. In particular, as shown in Fig.2c, when the wavelength, $\lambda$, is equal to 1.92$a$, an almost gap (a pseudogap) is formed; finally, at $\lambda$ around 1.25$a$, a true narrow gap is created (gap over midgap approximately 5%). This is a general feature of all known PCs: Gaps appear, if at all, when the photon wavelength is comparable to the spatial periodicity and the other characteristic lengths of the structure.

**Design and fabrication of photonic crystals**

In the 15 years since the initial idea[1,2] of creating spectral em gaps in periodic media, photonic crystals have developed into an emerging technological field[7] offering the possibility of manipulating the emission, propagation, splitting, switching focusing, etc of em waves. In other words a novel tool has been added to facilitate perhaps our quest for the holy grail of all-photon telecommunications.

The creation of a spectral em gap requires the strong periodic spatial modulation of the dielectric function, $\varepsilon$, and/or the magnetic permeability, $\mu$. This can be achieved by constructing composite materials consisting of two or more components with widely different $\varepsilon$ and $\mu$. Usually, at high frequencies, $\mu$ is close to one for most (if not all) materials. Thus we are often left with the dielectric function $\varepsilon$ as the only available material parameter. For the time being let us restrict ourselves to practically lossless dielectrics (although metals have also been used in the fabrication[6] of PCs). The simplest possible conceptual design of a photonic crystal is a composite consisting of spherical dielectric particles of high dielectric function ($\varepsilon = \varepsilon_2$) placed periodically in a dielectric matrix[3] of low dielectric function ($\varepsilon = \varepsilon_0$). The larger the ratio of dielectric functions, the stronger the scattering of em waves by the particles, and hence, the better the chances for gaps creation. Strong scattering is also promoted when the so-called Mie resonance conditions are satisfied, i.e. when the wavelength, $\lambda$, inside the particles is almost equal[3] to their diameter, $d$.

In order for the strongly scattered waves to interfere destructively, the periodicity based Bragg condition must also be satisfied leading to the relation $\lambda = 2a$. These considerations justify our previous observation, that gaps appear, if at all, when the photon wavelength is comparable to both the period of the structure and the diameter of the scatterers. Thus to have gaps in the near infrared or at optical frequencies we need three-dimensional structures with spatial period in the micron or the submicron range respectively. Furthermore, the Mie and the Bragg conditions lead usually to volume fractions occupied by the high $\varepsilon$ material of around 20%.

Several design parameters may influence the occurrence or not of gaps. We already mentioned the ratio $\varepsilon_2/\varepsilon_0$ (which must exceed 4.5) and the volume fraction, $f$, of the high $\varepsilon$ material. Other parameters are: the lattice structure formed by the centers of the inclusions; the shape of the inclusions; the topology, i.e. whether each inclusion is fully surrounded by the host material (cermet topology) or whether the inclusions are connected with each other to form a continuous network (network topology).

Regarding the lattice structure one expects that the fcc symmetry would be the favorable one for gap formation. The argument goes as follows: In any arbitrary direction of propagation there are always gaps; if these gaps were independent of the direction (as in the case of the non-realizable spherical symmetry), we would have a full all-direction gaps; then fcc, being as close to spherical symmetry as it is possible for a periodic structure, must be the preferable symmetry. Detailed calculations and experiments with acoustic (scalar) and elastic (full vector) waves confirmed this prediction. However, em waves surprised the researchers: it turned out[8,9] that diamond and diamond-like symmetry was the more favorable for em gap formation. There is no convincing explanation for this unexpected result, which may stem from the pure transverse nature of em waves and the consequent absence of a spherically symmetric scattered wave. Another odd behavior of em waves is related to the topology: In contrast to acoustic and elastic waves, the network topology, and not the cermet one, is the more favorable for em gap formation.

As the possible applications of photonic crystals grow, there is a proliferation of materials[6,7] and fabrication techniques[5-7,10] employed for their construction[6]: Thus semiconductors (Si, Ge, GaAs, AlGaAs/GaAs), oxides (SiO$_2$, TiO) polymers (PMMA), protein crystals, metals, and other materials have been used as components or templates for PC fabrication. For the latter lithographic methods (using e-beams, focused ion beams, femtosecond laser pulses, x-ray beams, holographic lithography) as well as self-assembled colloidal approaches combined with chemical etching have been employed. Extensive work has been devoted to the fabrication, study, and possible applications of two-dimensional photonic crystals[5,6] which allow easy design and construction of various devices, such as splitters, switches, etc.
It must be pointed out that the design of PCs and PC based devices is greatly facilitated by numerical solutions of Maxwell's equations in these systems, based on various theoretical approaches such as plane wave expansions, transfer matrix techniques, multiple scattering methods, and finite difference time domain (FDTD) discretization. These computations involve neither uncontrollable approximations nor adjustable parameters; consequently they are very reliable, being in excellent agreement with experimental data as the example of Fig.3 shows.

In Fig.4 we show examples of two PCs which have pushed the midgap frequency to the near infrared or almost optical range by quite different fabrication techniques. The layer by layer structure[11] (Fig.4a) was recently miniaturized[11] to micron length to produce a gap at telecommunication frequencies (i.e. wavelength of about 1.5 µ). The inverse opal structure[10,6] has naturally a lattice constant in the submicron range; however this important advantage makes the infiltration procedure by a high index dielectric difficult.

**Photonic crystals as negative (refractive) index materials (NIMs)**

Thirty five years ago, Veselago, a Russian physicist examined theoretically[12] what would happen to em waves propagating in a dispersive medium for which both μ(ω) and ε(ω) are negative and real. He found that the triad k, E, H is left-handed and not right-handed as in the usual case. As a result, the wavevector k and the Poynting vector $S = cE \times H / 4\pi$ are opposite to each other, which means that energy and phase propagate in opposite directions. Consequently, the em wave refracted at the interface of an ordinary medium and a negative ε, μ medium is in the “wrong” quarter plane as shown in Fig.5. This follows immediately by the conservation of energy and the parallel component of the wavevector and is equivalent to choosing the negative sign in the definition of the index of refraction as the square root of the product ε times μ (when both are negative). For this reason, materials with both ε and μ negative are referred to as negative index materials (NIMs) or left handed materials (LHMs), while ordinary dielectrics are called positive index materials (PIMs) or right handed materials (RHM). The negative refraction permits the construction of flat lenses made from a slab of NIM, if such material can be found. Recently, Pendry[13] proposed a composite structure (consisting of metallic split rings which act as magnetic resonators and wires which act as electric resonators) for which effectively both ε and μ have negative values (over a limited frequency range). Subsequently, Shelby et al.[14] constructed Pendry’s structure and demonstrated experimentally negative refraction. Furthermore, Pendry (see p.329 in ref.6) argued that a slab of NIM can, under certain conditions, act as a superlens in the sense that it can focus more accurately than the wavelength limit (by “magnifying” the evanescent components which are usually lost).

Such a drastic extension of a field as established and “final” as electromagnetism has raised various objections which can be summarized as follows:

(a) Superlensing is not possible.
(b) Negative refraction seems to violate parallel momentum conservation, since momentum is parallel to S.
(c) Fermat’s principle of minimum optical path is violated.
(d) Either negative refraction does not take place or causality and the speed of light is violated (because the outer ray of a beam of finite width has to move with infinite velocity in order to catch up with the inner ray in a negative refraction situation).
(c) Absorption (which is always present, since Pendry's resonators are metallic) would invalidate Veselago's conclusions.

The jury's verdict regarding the first objection is not yet out; existing numerical results and analysis suggest that probably the superlensing, although real, would not be very significant.

The second objection is baseless, since in a dispersive medium the momentum is not parallel to $S$; as a matter of fact in NIM the momentum is parallel to $k$.

The third objection is also groundless since Fermat's principle refers to the extremum (and not necessarily to the minimum) of the optical path.

Finally the last two objections can be addressed more conveniently by invoking photonic crystals, since they are inherently lossless and—by proper choice of their structure and the frequency range—can exhibit negative refraction index behavior [15] in the following sense: The Poynting vector (averaged over the time period and the unit cell), which is parallel to the group velocity, can be antiparallel to the crystal wavevector $k$; under these circumstances the sign of the refraction index is negative.

Recently Foteinopoulou et al. [15] considered a two-dimensional photonic crystal consisting of dielectric rods of radius $r = 0.35a$ and dielectric function $\varepsilon = 12.96$ placed in a hexagonal lattice of lattice constant $a$. In the range $a/\lambda$ between 0.57 and 0.61 the effective index of refraction is negative. A finite line source of em waves placed at an angle of 30 degrees relative to the interface between the vacuum and the PC starts emitting almost monochromatic radiation at $\lambda = 1.73a$ (corresponding to PC refractive index equal to $-0.7$); the inner ray of which reaches the surface of the PC after a time interval of $\Delta t = 0.56a/s$, while the outer one after $\Delta t' = 2.56a/s$, where $a/s = 1.5\lambda/c$.

The results of numerically following the evolution of the em wave as a function of time is shown in Fig.6a. The wave is trapped temporarily near the interface initially without indications of a specific direction of propagation (Fig.6a). Gradually signs of propagation along the direction determined by Snell's law (corresponding to the refractive index equal to $-0.7$) are shown (Fig.6b) and eventually after a long time (Fig.6c) this direction is clearly followed. This numerical calculation not only demonstrated negative refraction; it has also shown that it takes a relatively long time for the wave to reorganize itself near the interface and to establish eventually a steady state consistent with Snell's law and negative refractive index. Thus the simplistic zero delay ray picture, on which the fourth objection was based, is not at all relevant to what really happens at a PIM/NIM interface as an em wave hits it.

In conclusion, the artificial periodic structures called photonic crystals have opened up new horizons in a subject as mature as the electromagnetic wave propagation in materials; in addition they constitute an emerging technological field which may play a significant role in future telecommunications.

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References
The scope of Complexity

Long after the discovery of atoms and molecules it was still customary in science to think about a collection of many similar objects in terms of some "representative individual" endowed with the sum, or average of their individual properties. With the exception of particles physics and condensed matter theory where renormalisation group effects were fully recognised, scientists in various disciplines continued their research within the "mean field" framework.

In fact, one may argue that this "mean field" / continuum / linear way of thinking is what conserved the classical sciences as independent sub-cultures. Indeed, the great conceptual jumps separating the various sciences and the accompanying paradoxes connected to the nature of life, intelligence, culture arise exactly from the failure of these assumptions. When "More Is Different" life emerges from chemistry, chemistry from physics, conscience from life, social conscience/ organisation from individual conscience etc. (The title of the present article associates the beginnings of complexity with the article "More Is Different" published 30 years ago by Phil Anderson [1]).

This study of the emergence of new collective properties qualitatively different from the properties of the "elementary" components of the system breaks the traditional boundaries between sciences: the "elementary" objects belong to one science—say chemistry—while the collective emergent objects to another one—say biology. As for the methods, they fall "in between": in the "interdisciplinary space". The ambitious challenge of the Complexity research (its "manifest destiny") is prospecting, mapping, colonising and developing this "interdisciplinary" territory [2]. For a visual impression of the fields and subjects involved in the synthesis that complexity tries to achieve see Fig. 1.

Theoretical and phenomenological origins of complexity

Many of the crucial ingredients of Complexity appeared in the context of theoretical physics. In fact Anderson listed as his preferred examples phenomena which take place in physical systems: superconductivity, superfluidity, condensation of nucleons in nuclei, neutron stars, glasses.

He emphasised that in spite of the fact that microscopic interactions in the above phenomena are very different they can be all explained as realisations of a single dynamical concept: Spontaneous Symmetry Breaking. Therefore, the mere fact that various phenomena fall superficially in different empirical domains should not discourage scientists to study them within a unified conceptual framework [3]. This birth gift of an extreme unifying potential haunted in the intervening 30 years the Complexity research as its main blessing and curse.

Discreteness and autocatalicity as complexity origins

The discrete character of the individuals turned out to be crucial for the macroscopic behaviour of complex systems. In fact, in conditions in which the (partial differential) continuum approach would predict a uniform static world, the slightest microscopic granularity insures the emergence of macroscopic space-time localised collective objects with adaptive properties which allow their survival and development [4].

The exact mechanism by which this happens depends crucially on another unifying concept appearing ubiquitously in complex systems: auto-catalytic. The dynamics of a quantity is said to be auto-catalytic if the time variations of that quantity are proportional (via stochastic factors) to its current value. It turns out that as a rule, the "simple" objects (or groups of simple objects) responsible for the emergence of most of the complex collective objects have auto-catalytic properties.

Autocatalytic insures that the behaviour of the entire system is dominated by the elements with the highest auto-catalytic growth rate rather than by the typical or average element [5].
This explains the conceptual gap between sciences: in conditions in which only a few exceptional individuals/events dominate, it is impossible to explain the behaviour of the collective by plausible arguments about the typical or “most probable” individual/event. In fact, in the emergence of nuclei from nucleons, molecules from atoms, DNA from simple molecules, humans from apes, there are always the un-typical cases (with accidentally exceptional advantageous properties) that carry the day.

**Autocatalytic stochastic growth and power laws**

One of the early hints of complexity was the observation in 1897 by Pareto that the wealth of individuals spreads over many orders of magnitude (as opposed to the size of a person which ranges roughly between 1/2 metre and 2 metres). The dynamics of the social wealth is then not dominated by the typical individual but by a small class of very rich people. Mathematically one realised that instead of the usual fixed scale distributions (Gaussian, exponential), the wealth follows a “power law” distribution [6]. Moreover, in spite of the wide fluctuations in the average wealth during crises, booms, revolutions, the exponent of the power laws has remained between narrow bounds for the last 100 years.

Similar effects were observed in a very wide range of measurements: meteorite sizes, earthquakes, word frequencies and lately internet links. In all these systems, the presence of power laws constitutes a conceptual bridge between the microscopic elementary interactions and the macroscopic emergent properties. It turns out that the autocatalytic character of the microscopic interactions governing these systems can explain this behaviour in a generic unified way: by taking the logarithm of the variables, random changes proportional to the present value become random additive changes. This brings auto-catalytic dynamics within the realm of statistical mechanics and its powerful methods can be applied efficiently [7].

**The language of dynamical networks**

The unifying power of the Complexity view is expressed among other in the emergence of a common language which allows the quick, effective and robust/durable communication and cooperation between people with very different backgrounds. One of these unifying tools is the concept of dynamical network [8].

Indeed, one can think about the “elementary” objects (belonging to the “simpler” level) as the nodes of the network and about the “elementary” interactions between them as the links of the network. The dynamics of the system is then represented by (transitive) operations on the individual links and nodes ((dis)appearance, substitutions, etc.).

The global features of the network correspond to the collective properties of the system that it represents: (quasi-)disconnected network components correspond to (almost-)independent emergent objects; scaling properties of the network correspond to power laws, long-lived (meta-stable) network topological features correspond to (super-)critical slowing down dynamics. In this way, the mere knowledge of the relevant emerging features of the network might be enough to devise methods to expedite by orders of magnitude desired processes (or to delay or stop unwanted ones). The mathematical tools implementing it are developed presently and include multi-grid and cluster algorithms.

**Multigrid and clusters**

The mathematical counterpart to the physicist’s Renormalisation Group is the Multigrid tradition. In the last decade the two have interacted profitably and their relative strengths and weaknesses were complemented. A direction with a particular conceptual significance is the Algebraic Multigrid [9].

The Algebraic multigrid basic step is the transformation of a given network into a slightly coarser one by freezing together a pair of strongly connected nodes into a single representative node. By repeating this operation iteratively, Algebraic Multigrid ends up with nodes which stand for large collections of strongly connected microscopic objects. The algorithmic advantage is that the rigid motions of the collective objects are represented on the coarse network by the motion of just one object. One can separate in this way the various time scales. For instance, the time to separate two stones connected by a weak thread is much shorter than the time that it takes for each of the stones to decay to dust. If these two processes are represented by the same network then one would have to represent time spans of the order of millions of years (typical for stone decay) with a time step of at most 1 second (the typical time for the thread to break). The total number of time steps would become unacceptably large. The Multi-grid procedure allows the representation of each sub-process at the appropriate scale. At each scale the collective objects which can be considered as “simple” elementary objects at that scale are represented by just one node. This is a crucial step whose importance transcends the mere speeding up of the computations. By labelling the relevant collective objects at each scale, the algorithm becomes an expression of the understanding of the emergent dynamics of the system rather than a mere tool towards acquiring that understanding. Multigrid (and their cousins—Cluster) algorithms have the potential to organise automatically the vast amounts of correlated information existing in complex systems such as the internet, NMR data, etc.

**Particular Examples**

Much of the present Complexity work may be thought of as an application (with appropriate adjustments) of the table proposed 30 years ago by Anderson where the “simpler” science appears in the second column and the “more complex” one in the first:

<table>
<thead>
<tr>
<th>Atomic physics</th>
<th>elementary particles</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemistry</td>
<td>Atomic physics</td>
</tr>
<tr>
<td>Molecular Biology</td>
<td>Chemistry</td>
</tr>
<tr>
<td>Cell Biology</td>
<td>Molecular Biology</td>
</tr>
<tr>
<td>Psychology</td>
<td>Physiology</td>
</tr>
<tr>
<td>Social Sciences</td>
<td>Psychology</td>
</tr>
</tbody>
</table>

Below is an incomplete list of particular complexity directions substantiating this table. Of course, when looking for complexity one should keep in mind that “when you carry a hammer, a lot of things look like nails”. Some things might still be simple.

**A) Society**

The emergence of traffic jams from single cars

The traffic simulation is an ideal laboratory for the study of complexity: the network of streets is highly documented and the cars
motion can be measured and recorded with perfect precision. Yet the formation of jams is a very non-trivial consequence of the individual car events. Simpler, but not less important projects might be the motion of masses of humans in structured places, especially under pressure (in stadiums as a match ends, or in theatres during alarms). The social importance of such studies is measured in many human lives (see http://www.helbing.org and references therein for further information).

From customers to markets
The traditional approach in the product diffusion literature, is based on differential equations and leads to a continuous sales curve. This is contrasted with the results obtained by a discrete model that represents explicitly each customer and selling transaction. Such a model leads to a sharp (percolation) phase transition that explains the polarisation of the campaigns in hits and flops for apparently very similar products and the fractal fluctuations of the sales even in steady market conditions [10].

The emergence of financial markets from investors
The financial economics has a long history of using precise mathematical models to describe the market behaviour. However, in order to be tractable, the classical market models (the Capital Asset Pricing Model, the Arbitrage Pricing Theory, the Option Valuation Black-Scholes formula) made assumptions which are found invalid by the behavioural finance and market behaviour experiments. By using the direct computer representation of the individual investors' behaviour, one can study the emergence of the (non-equilibrium) market dynamics in the presence of completely realistic conditions [11]. The simulations performed until now have already suggested generic universal relationships which were abstracted and then taken up for theoretical study in the framework of stylised models [12].

Interactive markets Forecast and regulation
After loosing a fortune in a bubble (triggered by the South Sea Co.) in 1720 at the London Stock, Sir Isaac Newton was quoted to say: "I can calculate the motions of the heavenly bodies, but not the madness of people." It might seem over-ambitious to try where Newton has failed but let us not forget that we are 300 years later, have big computers and have had plenty of additional opportunities to contemplate the madness of people.

Understanding and regulating the dynamics of the (financial) markets is in some ways similar to predicting and monitoring weather or road traffic, and at least as important: One cannot predict individual car accidents but one can predict based on the present data the probable behaviour of the system as a whole. Such prediction ability allows the optimisation of system design as well as on-line intervention to avert unwanted disturbances etc. Moreover one can estimate the effect of unpredictable events and prepare the reaction to them.

It is certainly a matter of top priority that the public and the authorities in charge of economic stability will have at their disposal standard reliable tools of monitoring, analysis and intervention [11].

Horizontal interaction protocols and self-organised societies
The old world was divided in distinct organisations: some small (a bakery, a shoe store) and some large (a state administration, an army).

The way to keep it working was for the big ones to have a very strict hierarchical chain of command and for the small ones (which couldn't support a hierarchy) to keep everybody in close "horizontal" personal contact. With the emergence of the third sector (public non-profit organisations), with the emergence of fast developing specialised activities, with the very lively ad-hoc merging and splitting of organisations, the need for lateral (non-hierarchical) communication in large organisations has increased. Yet, as opposed to the hierarchical organisation, nobody knows how to make and keep under control a non-hierarchical organisation. The hope is that some local protocols acting at the "local" level may lead to the emergence of some global "self-organising" order. The study and simulation of such systems might lead to the identification of modern " Hammurapi codes of laws" with which to regulate (and defend) the new "distributed" society.

B) Biology

The emergence of the Immune Self from immune cells
The immune system is a cognitive system: its task is to gather antigenic information, make sense out of it and act accordingly. The challenge is to understand how the system integrates the chemical signals and interactions into cognitive moduli and phenomena. Lately, a few groups adopted the method of representing in the computer the cells and enzymes believed to be involved in an immune disease, implement in the computer their experimentally known interactions and reactions and watch the emergence of (auto-)immune features similar with the ones observed in nature [13]. The next step is to suggest experiments to validate/amend the postulated mechanisms.

Identifying and manipulating the "atoms" of life
The situation in molecular biology, genetics and proteonics today resembles the situation of Zoology before Darwin and of Chemistry before the periodic table: "everything" is known (at least all the human genes), some regularity rules are recognised, but the field lacks an unifying dynamical principle. In particular the dynamics of "folding" (the process that gives the proteins their shape given a certain base sequence) and the relation between each protein shape and its function are anybody's guess.

In principle it is arguable that these problems can be solved within the borders of the present techniques and concepts (with some addition of data mining and informatics). However, I would bet rather on the emergence of new concepts, in terms of which this "total mess" would become "as simple" as predicting the chemical properties of elements in terms of the occupancy of their electronic orbitals. So the problem is: what are the "true" relevant degrees of freedom in protein/genes dynamics? Single bases / nucleic acids are "too small"; alpha chains or beta sheets—are too big. See the new ComplexUs journal www.karger.ch/journals/cpulcpujh.htm for relevant interdisciplinary efforts to solve this problem. Of course answering it will transform the design of new medicines into a systematic search rather than the random walk that is today.

C) Cognition

The emergence of perceptual systems
(the example of the visual system)
The micro-to-macro paradigm can be applied to a wide range of perceptual and functional systems in the body. The main steps are to find the discrete microscopic degrees of freedom, their elementary interactions and to deduce the emergent macroscopic degrees of freedom and their effective dynamics. In the case of the...
visual system this generic program is quite advanced. By using a combination of mathematical theorems and psychophysical observations one identified the approximate, ad-hoc algorithms that the visual system uses to reconstruct 3 D shapes from 2 D image sequences [14]. As a consequence, one predicted specific visual illusions that were dramatically confirmed by experiment. This kind of work can be extended to other perceptual systems and taken in a few directions: guidance for medical procedures, inspiration for novel technology, etc.

**Complexity induces a new relation between theoretical and applied science.**

The processes of drawing and handwriting (and most of the thought processes) look superficially continuous and very difficult to characterise in precise terms. Yet lately it was possible to isolate very distinct discrete spatio-temporal drawing elements and to put them in direct relation to discrete mental events underlying the emergence of meaningful representation in children [15]. The clinical implications e.g. for (difficulties in) the emergence of writing are presently studied. This realisation that there are intermediate (higher than neuron) scale “atoms” in the cognitive processes is very encouraging for the possibility to apply complexity methods in this field.

**Conceptual structures with transitive dynamics**

Dynamical networks were mentioned as a candidate for a “lingua franca” among complexity workers. The nodes are fit to represent system parts / properties while the links can be used to represent their relationships. The evolution of objects, production processes, ideas, can then be represented as operations on these networks [16].

By a sequence of formal operations on the initial network one is led to a novel network. The changes enforced in the network structure amount to changes in the nature of the real object. The sequence of operations leading to novel objects is usually quite simple, mechanical, well defined and easy to reproduce. It turns out that a handful of universal sequences (which have been fully documented) are responsible for the novelty emergence in nature. Incidentally, ideas produced by a computer that applied one of these sequences obtained (from double-blind humans) higher inventiveness marks than the ideas produced by (a second group of) humans.

**Conclusions**

The aim of Complexity is to express, explain and control the collective objects and phenomena emerging at a certain space-time scale from the simpler interactions of their components at a finer scale. This is a sort of extension of the stochastic “atomic-molecular” methods to social, biological and cognitive problems.

The interdisciplinary integration that this implies is not just a juxtaposition of various expertise but rather a much more intimate fusion of knowledge. It rather involves a coordinated shift in the very objectives, scope and ethos of the affected disciplines. Complexity is not offering just a way of answering a question from one science using concepts from another: it is introducing a new language which allows the formulation of novel questions or rather a new grammar which allows novel interrogative forms. Bringing people from these disciplines together is not enough. These fields have very different “cultures”: different objectives, criteria of success, techniques and language. A deep shift in their way of thinking is necessary.

To realise it requires “growing” a new generation of “bilingual” young scientists that will produce the necessary synthesis in their own minds.

Complexity induces a new relation between theoretical and applied science. In the past, as technology was acting on hardware objects, applied science was mainly experimental science applied to real life situations. Today, when technology is acting on information, applied science consists often of theoretical / abstract operations applied to real life information items. One may have to get used to the expression “Theoretical Applied Science”.

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**References**


Remembering Eugene Wigner and pondering his legacy

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When I looked into the 1992, November issue of Fizikai Szemle in which Wigner was celebrated on his 90th birthday, I saw the list of his well over 300 publications in all branches of physics, in chemistry and in pure mathematics. My first reaction was to withdraw from this attempt of doing him justice in a single talk. On some reflection I thought of a way out.

The early years

Wigner's life coincided with the 20th century. He was almost of the same "quantum age" as Heisenberg and Pauli, however, these two were in the center of the Copenhagen School and from 1925 on were among the main architects of quantum mechanics (QM). By contrast 1925 was the year when Wigner graduated as chemical engineer in Berlin. He must have felt way behind these pioneers, yet, he soon became one of the leaders of the new discipline. Moreover we shall see that his being rooted in chemistry sheds light on some of the subtler aspects of QM.

Michael Polanyi was among Wigner's mentors in chemistry. Their joint work on molecular reaction chemistry is one of the standard papers in the field. After obtaining his engineering degree Wigner returned to Budapest to work in the tanning factory where his father was director. He felt frustrated, but Polanyi came to the rescue with an invitation to Berlin to an assistantship in x-ray crystallography. Wigner resumed attendance at the physics colloquium and felt great attraction to QM. The factory had been a dead-end, but the chemical training and his sensitization to mathematics in school were positive influences, since QM was basically a novel confluence of physics, mathematics and chemistry.

Wigner drifted towards physics through a sequence of increasingly purposeful appointments. During this period the relation of the just mentioned disciplines changed radically and I will focus on Wigner's contribution to this change.

From chemistry to physics

Let me remind you of the status of chemistry at the time. The critical role of nitrogen fixation for the Central Powers' ability to pursue World War I was well known. Fritz Haber was awarded the chemistry Nobel Prize in 1918 for this achievement. At the time mathematics and physics did not seem like practical careers. The fathers of John v. Neumann and Edward Teller also directed their sons toward chemical engineering. Yet, all three moved from chemistry that seemed to them an empirical craft, toward a physics based on mechanics that was already penetrated by subtle mathematics. An alternative way to see this is that chemistry changed from being an empirical craft to a discipline increasingly intertwined with mathematical physics.

Wigner made considerable contributions to this process. His excellent chemical engineering training in Berlin prepared him for his role of designing the plutonium production facility in the Manhattan Project. The task was to upgrade traditional chemical engineering techniques to include nuclear phenomena, say, the novel cooling problems. This cooperative effort with chemical engineers turned Wigner into a pioneer of nuclear engineering.

Wigner's background helped shape his contribution to fundamental QM years before this event. His early experience in x-ray crystallography called his attention to symmetry. This resonated with his liking for mathematics stimulated by a favorite high school teacher Dr. Laszlo Ratz. His friend Johnny von Neumann substantially added to this orientation. All this culminated in a program of applying the theory of group representations to atomic spectroscopy. The papers that he wrote in 1927-9, some of them jointly with Neumann, are seminal in the field.

At that time most physicists disliked group theory, a sentiment expressed in the widely used "Gruppenpest". This parlance was not a whimsical expression of distaste, but had a philosophical background. Most classical physicists expected infinitesimal analysis to be the natural mathematics for all of physics, with priority accorded to the differential equations of Newtonian mechanics. It was a widely held tacit assumption that this must be the way mathematics enters microphysics. One of the reasons that QM is still not accepted with complete ease is that its most appropriate way to mathematics is different. Such a new way is provided by group theory. Although the important rotation group is continuous, the theory of group representations deals with a discrete substructure. It was Johnny von Neumann who alerted Wigner to this highly esoteric link between discrete and continuous mathematics and one of the non-Newtonian entry ports for mathematics into QM. This effort culminated in the book Group Theory & Application to the QM of Atomic Spectra, 1931. This work in German was translated into English in 1959 and appeared in many editions.

...how could Wigner make reliable contributions to so many subdisciplines of physics?
Although Wigner’s book was confined to atomic spectroscopy, he authored group-theory papers also on molecular spectra, solid state, nuclear physics and the infinite unitary representations of the Lorentz group. His contribution to symmetry, particularly in the context of nuclear physics was awarded the Nobel Prize in 1963. My lack of competence in nuclear physics and the vast number of papers keeps me from highlighting his principal achievements along these lines. However, it is not hard to hint how could Wigner make reliable contributions to so many subdisciplines of physics? His oeuvre was centered on chemistry made up of a hierarchy of levels: structure of atoms, molecules, crystals and nuclei and to some extent elementary particles. A precise and reliable mathematical description was given in terms of group theory. This vast collection of papers constitutes the bulk of Wigner’s legacy. Yet there is something else. QM has mysterious paradoxical aspects and there is no unanimity even as to the definition of the difficulties, let alone as to their removal.

Whereas the rules of experimental precision and mathematical rigor are well established, I believe that the rules for associating mathematics with experience are sufficiently ambiguous to give rise to paradoxes. This seldom-featured ambiguity is the butt of Wigner’s ironical musings in The Unreasonable Effectiveness of Mathematics in the Natural Sciences. (Comm. in Pure and Appl. Math. 13, No.1, 1960; reprinted in Wigner, Symmetries and Reflections, Indiana University Press, Bloomington & London, 1967, p 222.)

This is an often reproduced and widely read paper; it has great charm with an understated sense of humor. It is utterly free of technical jargon, but has a complex message, the first part of which is that “mathematics is effective in the natural sciences”. This message is undisputed but it is not new. It is more questionable why this effectiveness should be “unreasonable”? In the biography by Andrew Szanton to which Wigner generously contributed, a word count would seem to reveal the importance he assigned to what is “reasonable”. What should we make of the prominent use of “unreasonable” in the title of this paper?

Unreasonable theory

A theory will be deemed “unreasonable” if it conflicts with common sense imbedded in established tradition. Under such conditions one will place a new theory “on probation”. There were many theories that were emended or have fallen by the wayside and are happily forgotten. It is more interesting that occasionally “unreasonable” theories are stubbornly irrepressible. Think of the unreasonably moving earth of Copernicus.

After the new theory is sufficiently confirmed, it appeared that it is “common sense” that has to be harmonized with it, rather than vice versa. Nothing is so hard as modifying entrenched tradition and it is remarkable that mathematical physics excels in handling such situations. The heuristic foundation is then reclassified as temporary scaffolding that only hides the beauty of the façade. We can make use of the contrasting role of the scaffolding only if we recognize science as a two-stage process. In the heuristic stage the prime concern is to extend the frontier even at the price of contradiction and paradox. In the stage of consolidation, or rational reconstruction all paradoxes must be resolved and entrenched prejudices abandoned: the cathedral stands even as the scaffolding is removed. It is an entirely novel insight of scientific methodology that the logical standards in the two stages are very different.

Wigner was and remained ambivalent as to this issue, but we can filter out two inconsistent lines within his argument and examine the condition under which they could be reconciled with each other.

Quantum mechanics

Wigner sees that the superior qualities of QM are unaffected by the flaws of its foundations. He concludes on a cheerful note: “The miracle of appropriateness of the language of mathematics for the formulation of the laws of physics is a wonderful gift which we neither understand nor deserve. We should be grateful for it and hope that it will remain in future research and that it will extend, for better or for worse, to our pleasure, even though to our bafflement, to wide branches of learning.”

This is a “cheerful note” in the sense that it comforts the pioneer who was desperate to establish a new bridgehead even if he had to violate “common sense”. There was a time span of almost a century and a half between the masterpieces of Copernicus and Newton. The transitional figures of this period achieved their role only because they were able to operate in a logical twilight zone of contradictory notions. From the point of view of distant descendants the most interesting lesson of history is the struggle from the twilight zone into clarity by overcoming inherited dogma, the generator of paradox. This struggle can be turned into a paradigm that was to be replayed in a few instances. The outstanding example of the 20th century is Einstein’s special relativity (SRT). The significant difference from the Lorentz–Poincare theory is Einstein’s insight that Newtonian absolute time has only asymptotic validity. This followed from the postulated consistency of Newtonian mechanics and Maxwellian electrodynamics. Einstein recognized that the methodology of SRT is superior to that of QM. Although SRT strains our common sense notion of absolute time, Einstein taught us how to do without this notion for uncommon experiences.

By contrast, we haven’t yet learned to recognize the provincialism we have to keep under control to be comfortable with QM. According to a well-reasoned recent study, this discipline is no less paradoxical than ever. (See F. Laloe, Am. J. Phys, 69, 2001, p 655.) When Wigner was first introduced to QM, paradoxes were rampant; yet the theory was utterly convincing; hence Wigner’s acceptance of “unreasonable” methods. When he wrote this paper thirty years later, he had a secret hope that a sharpened method might lead to the resolution of paradoxes. I believe this secret hope may have been behind the mysterious motto of the paper: “…and it is probable that there is some secret here which remains to be discovered.” – C. S. Peirce.

Experience and mathematics

What else could be the “secret”, but a rational explanation of the “unreasonable” correspondence between experience and
mathematics. The apparent conflict between the two attitudes can be reconciled by realizing that the scientific enterprise is a composite of apparently opposite moves. The first heuristic penetration into a new area of knowledge calls for the free creative imagination of the discoverer, maybe defying common sense. The second stage of consolidation calls for the elimination of such conflicts.

To sum up, the architects of QM are to be credited with the creation of a flawless theory of atoms, molecules and the condensed state of matter, but the so-called “breakdown of classical physics” is a poor substitute for the actual separation of the classical theory into perennial and obsolete parts. The failure to remove the latter manifests itself as a “paradox” that was improperly attributed to a flaw of QM, whereas actually it is a flaw in the 20th century interpretation of classical physics. Whereas this interpretation may have been problematic at the beginning of the 20th century, after another century there should be no difficulty to handle the matter, assuming willingness to break with dogmatic thinking. The problem to be kept in mind is that Newton scholars have given well-deserved attention to the complications involved in the axiomatics for the mechanics of the Principia and to the paths that connect Newton with his predecessors. By contrast, little attention is given to Newton as the founder of all of mathematical physics and to the imperfections the successors have only partially corrected in building late classical physics.

I have recently addressed this question of consolidation in Tisza: The reasonable effectiveness of mathematics in the natural sciences, Experimental Metaphysics, R. S. Cohen, et al. (eds.), The Kluwer Publ. Co., 1997, pp. 213–238. The title is an obvious take-off on Wigner’s paper and my aim was to recognize behind its playful ambivalence Wigner as the champion of reason who was biding his time. Although my paper is rather lengthy, the underlying ideas are relatively simple and I will sum up the main points.

The basic axiom of Newtonian mathematical physics is stated in the Preface to the first edition of the Principia: rational mechanics ought to address “motion” with the same precision as geometry handles the size and shape of idealized objects. It is interesting, however, that the core of Newton’s method is also in line with Einstein’s preference for “theories of principle”. The association of “motion” with “mathematics” was a stroke of genius; but to appreciate its full impact, we must distinguish between the short-term and the long-term uses of this idea.

From Newton...

By producing the mechanics of the Principia Newton demonstrated that in the short-term there is a simple instance of motion, namely rigid translation that can be formalized in terms of available mathematics. Newton expected that his work would be effective also in the long-term. (The Third Rule of Reasoning in Philosophy, in Book III of the Principia. As an empiricist Newton added the Fourth Rule according to which this extrapolation is subject to experimental verification.)

It is a fact that the Third Rule exercised great attraction both for Einstein and Bohr. When Newtonian mechanics failed to account for the stability of the Rutherford atom, Einstein felt as if the ground were pulled from under him. Was this the end of the Newtonian epistemology? The epistemological discussions of the century are indeed marked by a tone of resignation. However looking back at the overall picture we see rather a vast explosion of knowledge. There was a retrenchment of expectations; but this is overshadowed by opening up new evolutionary avenues of exploration.

A century later we have every reason to bet on the evolutionary option. It is evident that the area of knowledge is being extended rather than narrowed. Instead of deploiring the breakdown overcome only by revolution, we should understand the rules of the new evolution opened up by using new mathematics and wider scope of the concept of motion.

The first significant advance beyond Newton was directed at the expansion of the mathematical base. The work of continental mathematicians active over a century and a half converged into a highly successful analysis of the continuum. They considered Newtonian mechanics as a natural proving ground for the new mathematics. This was an expression of preference over the dynamics of Descartes but a rejection of Newton’s Euclidean addiction; it led to an innovative analytical mechanics. The physics community accepted the innovation and called its Hamiltonian version canonical mechanics. This terminology implied, correctly, that a specific mathematical formalism might have a closer affinity to a theory of physics than alternative choices, even if one happens to be more familiar. Unfortunately, the term canonical is overstated; it is preferable to call the formalism optimal for Newtonian mechanics, but not to foreclose another choice for dealing with heat, light, electricity and magnetism, and for atomic physics.

The first one to break out of the canonical straight jacket was Faraday; he initiated an alternative approach, as all the listed non-mechanical phenomena can be also associated with the chemical structure of the atom. Maxwell’s translation of Faraday’s qualitative theory of the electromagnetic field into a mathematical formalism became an accepted branch of classical physics. This innovation was accepted by Einstein who stressed that the diversification of classical physics has to be met by consistency conditions. The requirement that Newtonian mechanics and Maxwellian electrodynamics be mutually consistent calls for the scrutiny of the concept of simultaneity and leads to the foundation of special relativity.

... to Einstein

Einstein emphasized that his method of transcending classical physics is logically flawless and he hoped that QM could be handled similarly. I suggest that this is a sensible program. Faraday’s chemical departure goes much beyond the electromagnetic field and marks a bifurcation in the evolution of classical physics into a mechanical and a chemical branch that calls for the formulation of another consistency relation.

Whereas in case of SRT the sensitive concept was absolute time, in the case of QM there is a different particle concept implicit in Newtonian mechanics and in Faraday’s chemical departure. Faraday’s chemical atom was different from the mechanical atom implicit in Newtonian mechanics. The mechanical atom is defined by its position and velocity; it has no intrinsic structure. Two observations refer to the same particle if the observations refer to points on the same orbit as for the evening star and the morning star. By contrast, the chemical atom has intrinsic structure and
different sample of the same structure form a class of indistinguishable particles, regardless of position.

Real particles have both mechanical and chemical properties and it is the uncertainty principle that ensures their mutual consistency. The Heisenberg principle restricts the scope of the mechanical measurement; the overall power of measurability is increased due to the emergence of the chemical branch. This becomes apparent in the context of the extraordinary junction in 1859 when Bunsen and Kirchhoff joined chemical analysis with spectroscopic measurements. The discovery that all the stars are made of the same elements we find on earth was easily the largest extension of knowledge ever attained in a single step.

At exactly this time the concept of molecular mean free path was established which led to the kinetic gas theory. The bifurcation of physics into mechanical and chemical branches was firmly in place. Accordingly, it is misleading to speak of the breakdown of classical physics; we have to differentiate between the two branches. The fact that the application of Newtonian mechanics fails to explain the observed stability of a discrete set of states of the nuclear atom, indicates the failure of mechanical classical physics on the atomic level. By contrast, the Bunsen- Kirchhoff landmark indicates a great expansion of the scope of the chemical branch. It led through Planck to quantum theory and on to QM.

Although the bare facts of the discovery of spectral analysis are well known, not enough is made of the epistemological revolution involved that marks a vast enrichment of the methods of acquiring knowledge.

I claim that such an epistemological principle is implicit in the Bunsen–Kirchhoff spectrum analysis. In this procedure light beams replaced the chemical reagents of traditional qualitative analysis. Light beams travel unimpeded though space and therefore the junction of chemical and optical methods vastly expand what these methods could achieve on their own. This is connected with an entirely new conception of measurement. It is very different from the Newtonian prediction that is vulnerable to any randomness. The light beam emerging from the diffraction grating consists of a random stream of photons yet leads to an accurate inference of the photon energy. This answers Einstein’s concern that God does not play dice with us.

This answers Einstein’s concern that God does not play dice with us.

widespread interpretation preferred reduction of chemistry to mechanics.

This expectation collapsed when Newtonian mechanics failed to account for the stability of the nuclear atom. What actually happened was a consistent joint use of the disciplines and the particle concept of QM is in closer harmony with chemistry than with mechanics.

I am glad to see that Hungarian education tends to unify basic chemical experience, such as the Periodic Table, quantum states, chemical bonds with fundamental atomic physics. (George Marx, Physics Education, September–November 1976, Institute of Physics, UK.)

Remembering E. Wigner

I wish to conclude on a personal note. I did not belong to Wigner’s circle of intimate Hungarian friends, but our paths crossed since the beginning of my life in physics. I was a mathematics student in Budapest and Göttingen, where I attended Max Born’s first ever course on quantum mechanics. I was impressed that higher mathematics found application to subtle empirical problems and—somewhat hesitantly—considered changing from mathematics to mathematical physics. This was the background when on vacation in Budapest I got an unexpected invitation for tea from Eugene Wigner. By that time, 1929, he was already a foremost theorist; the difference in our status was staggering. The invitation was an indication of the kindness and helpfulness of Eugene, for which he was well known. This invitation helped me overcome my timidity in making my important decision.

To return to the present, beyond my limited personal contacts I was also engrossed with Wigner’s style of insisting on the integrity of mathematics, no less than its empirical adequacy. I hope that this affinity ensures my credentials to interpret an aspect of his work that he left ambiguous. Traditional principles refuted by experiment must be abandoned. This does not call for a revolutionary break with the past. At this late stage tradition is likely to be only slightly out of focus, the flaw of tradition is to be removed by careful analysis. The required methods were not available at the turn of the 20th century and the empirically all but perfect QM seemed paradoxical from the perspective of an obsolete tradition. We ought to remove the paradoxes of QM not by changing this theory, but by removing the obsolete part of classical physics. From my familiarity with Wigner’s work, I feel that his understated alternative of pursuing C. S. Peirce’s “secret” comes closer to his real views than the apparently flippant endorsement of the freewheeling use of paradoxes to support subjective beliefs.

If my analysis of the situation would in any way contribute to a critical review of ancient preconceptions, I am confident that Eugene would endorse my role as his mouthpiece.

Acknowledgements

I wish to thank Abner Shimony for discussions, particularly on the background in which the paper in question came about. Wigner thanks him for the reference to Peirce, but Abner tells me that the selection of the motto was Wigner’s. It was important to him. I also thank George Marx for informing me about current trends in Hungarian education.
Digital in-line holography

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In his 1948 paper *A New Microscopic Principle* Dennis Gabor[1] points out that ‘It is known that the spherical aberration of electron lenses sets a limit to the resolving power of electron microscopes at about 5\(\AA\).... Prospects of improvement are... aggravated by the fact that the resolution limit is proportional to the fourth root of the spherical aberration.’ He continues ‘The new microscopic principle described below offers a way around this difficulty, as it allows one to dispense altogether with electron objectives.’ He called it ‘electron interference microscopy’ what later became holography.

The principle of holography is most easily explained with Gabor’s original implementation as illustrated in Figure 1. A spherical wave of wavelength \(\lambda\) emanating from a ‘point’ source of linear dimensions of the order of the wavelength, illuminates an object, typically a distance of a few thousand wavelengths from the source, and forms a highly magnified diffraction pattern on a screen much further away, see Fig. 1. We denote by \(A(r,t)\) the wave amplitude (the wave function for electrons or the electric field vector for photons) and split it into the unscattered reference wave, \(A_{ref}(r,t)\), and the wave, \(A_{scat}(r,t)\), scattered by the object. Ideally the reference wave emanating from the source is a spherical wave, \(A_{ref}(r,t) = \exp(ikr)/r\) where \(k = 2\pi/\lambda\) is the wave number. In an experiment this spherical wave is modified by the emission cone of the source. However, this can be accounted for by constructing, from the intensity, \(|A(r,t)|^2\), the contrast image

\[
\bar{I}(r) = |A_{ref}(r,t) + A_{scat}(r,t)|^2 - |A_{ref}(r,t)|^2
= |A_{ref}(r,t)A_{scat}(r,t) + A_{ref}(r,t)A_{scat}^*(r,t)|^2
+ |A_{scat}(r,t)|^2 \quad (1)
\]

We will refer to the first term (in brackets) in (1), linear in the scattered wave, as the ‘holographic diffraction pattern’ because it arises from the superposition of the interference terms between the unscattered reference wave from the source and the scattered wave from the object. The second term in (1) contains the interference between the scattered waves. We will refer to it as the ‘classical diffraction pattern’. Holographic diffraction dominates the images for small objects; loosely speaking ‘small’ means that the object should only block a fraction of the cone of radiation recorded on the screen. Even if these objects are opaque, we are still in the regime of holography, and will be able to recover the outline or shape of the object. As the scattered wave amplitude grows because more of the incoming reference wave is blocked out by larger objects, classical diffraction becomes more important. When it eventually dominates the image, we are in the regime of classical wave optics.

A hologram is just a complicated interference pattern from which little information about the shape and structure of the object can be obtained by simple inspection. What object, as an example, produced the hologram in panel (a) of Fig. 2? Holography was therefore conceived by Gabor as a two-step process: first, a hologram must be recorded, and second, reconstruction must yield an ‘image’ of the object, i.e. the intensity of the scattered wavefront at the object. The reason why the second step is possible is the fact that the holographic information is linear in the scattered wave so that an inversion of the scattering process is feasible. This, Gabor envisaged, could be achieved by recording the hologram photographically on a transparent plate and then ‘looking’ through the hologram from the back. As Gabor put it: ‘One must expect that looking through such a properly processed diagram one will see behind it the original object, as if it were in place.’ Gabor tested this idea with visible light but the quality of the reconstruction was not overwhelming. More importantly, the application in electron microscopy needed modification for two reasons: (1) A photographic plate is not transparent to electrons, and (2) using the same wavelength for the reconstruction would not yield any magnification. Therefore Gabor suggested to use visible light for the reconstruction after scaling up all dimensions in the ratio of light waves to electron waves, that is, by about a factor 100,000.

Although attempts at electron holography were made early on, their success was very limited, essentially because the condenser lenses for electrons at the time were so poor that no focus of the size of the electron wavelength of much less than angstroms could be achieved. A breakthrough came in the late 1980’s when Fink and collaborators showed that an ultrathin metal tip with one or a few atoms at its apex serves as a ‘point’ source with a virtual source size of atomic dimensions for a coherent beam of electrons with energies in the 10-200eV range. A new kind of microscopy with point sources, now called Low Energy Electron Point Source (LEEPS) microscopy, evolved from combining the technological tools of scanning probe microscopy with new ideas in projection microscopy. We refer the reader to a recent review article with further details and references.[2]

In the optical realm holography took off in the early 1970’s after the availability of lasers. Although holography with spherical waves, as originally proposed by Gabor and now called in-line holography, is the simplest realization of the holographic method, because it works without lenses, its applications had been limited until recently due to the fact that reconstruction of the object image with another wave is not practical. To avoid this problem various schemes of off-line holography have been developed in which a laser beam is split to provide an undisturbed reference wave while the other beam is focussed onto the object. There are too many variations on this scheme to allow an adequate overview here and the reader is referred to two books[4, 5] in which the principles and the practical implementations are described in detail. The remainder of this article will deal exclusively with our work on digital in-line holography with numerical reconstruction.1

In digital in-line holography—DIH—the hologram is recorded by a detector array, such as a CCD camera for photons, and transferred to a computer in which the reconstruction is done numerically. The role of reconstruction is to obtain the three-dimensional structure of the object from the two-dimensional hologram on the screen, or, in physical terms, to reconstruct the
in which the integration extends over the two-dimensional surface of the screen with coordinates $\xi = (X, Y, L)$ where $L$ is the distance from the source (pinhole) to the center of the screen (CCD chip); and $I(\xi)$ is the contrast image (hologram) on the screen obtained by subtracting the images with and without the object present. The function $K(r)$ is significantly structured and different from zero only in the space region occupied by the object. By reconstructing the wave front $K(r)$ on a number of planes at various distances from the source in the vicinity of the object, a three-dimensional image can be built up from a single two-dimensional hologram. $K(r)$ is a complex function and one usually plots its magnitude to represent the object, although phase images are also available. For the numerical implementation of the transform we have developed a fast algorithm that evaluates $K(r)$ without any approximations. It is incorporated in a self-contained program package, originally developed for electron holography, called LEAPS, that not only performs the numerical reconstruction but also all other procedures connected with data management and visualization [7].

In holography, the term ‘reconstruction’ is used to obtain the function $K(r)$ from the hologram. The plot of $|K(r)|$ on a two-dimensional plane, which we will call a 2-D holographic reconstruction, perpendicular to the optical axis is equivalent to one in-focus image taken in a conventional compound microscope. In DIH one can generate a stack of 2-D holographic reconstructions from a single hologram. Combining such a stack will result in a three-dimensional image of the object; this latter step is usually referred to as 3-D reconstruction.

The experimental setup for optical DIH, following the schematic of Fig. 1, is very simple: a laser is focussed onto a pinhole, of a diameter of the order of the wavelength, which acts as the “point source” from which a spherical wave of wavelength $\lambda$, emanates. The wave illuminates an object, in our setup a few millimeters from the pinhole, and forms a geometrically magnified diffraction pattern on a screen, in our case a CCD chip, a few centimeters away. If the scattered wave, shown by dotted line in Fig. 1, from the object is small compared with the unscattered reference wave, the interference pattern on the screen constitutes a hologram, linear in the scattered wave. The hologram is stored as a digital image in a computer for reconstruction.

To establish DIH as a new microscopy it is important to make detailed comparisons between images from conventional compound light microscopy and those obtained with DIH. For this purpose we used a setup in the lower panel of Fig. 1 in which a standard inverted compound microscope is used to obtain a digital record of the bright-field image seen through the ocular in the normal way. To record a hologram of the same sample area, a pinhole (typical diameter 1-5 $\mu$m) was placed between the objective lens and the sample such that the spherical light waves from the pinhole passed through the selected sample area. The laser light that illuminated the pinhole was introduced through a side port in the microscope and was directed towards the objective lens and pinhole via a movable mirror. The hologram was recorded with a CCD camera that was supported on the microscope work plate and centered over the pinhole and the selected area of the sample. The distance of the CCD camera from the pinhole, typically a few centimeters, was adjusted to capture all interference fringes of the hologram that could be resolved with enough pixels. The pinhole was mounted on an X-Y micrometer stage and could be moved out of the way to image the sample in bright field. As we mentioned above the input to the reconstruction formula (2) is the contrast image for a perfectly spherical incoming wave. It transpires that perfecting this image is the hardest part in the practical implementation of DIH. Guided by the experience in photoelectron and LEED holography we have implemented the following procedure:

(i) Record digitally the hologram of the object, giving a matrix $I_m$ of the intensity recorded on the CCD chip, where $n$ and $m$ enumerate the pixels in the x- and y-directions.

(ii) Remove the object and record digitally the intensity matrix $I_m^{00}$ of the illuminating laser.

(iii) Construct numerically the contrast image, corrected for the intensity variations in the primary laser beam, $I_m = (I_m - I_m^{00})/N I_m^{00}$. By this procedure almost all imperfections in the laser source are eliminated. Indeed, this step minimizes the quality requirements on the laser itself, as long as the laser is sufficiently stable to capture identically both images. We have checked this by comparing the contrast images obtained with (i) a high quality laser and (ii) a cheap laser pointer. The results in reconstruction are of comparable quality.

The contrast image, an example is given in panel (b) of Fig. 2, is next used in the reconstruction algorithm, based on the transform (2), to produce a series of 2-D holographic reconstructions at different distances from the source, i.e., the pinhole. Because the source-object distance can be measured directly with an accuracy of only a millimeter or so, it is necessary to zoom in with a series of reconstructions at different distances, displayed in the LEAPS program package as a film, to achieve accuracy at the submicron level.

As a first application we show, in panel (c) of Fig. 2, the reconstruction of the hologram in panel (b): it is an image of a Scanning Tunneling Microscope tip, the end of the tip has a diameter of less than 1 $\mu$m.

To demonstrate the state of the art in optical DIH we show in Fig. 3 holograms and images of latex microspheres having a mean diameter of 1 $\mu$m. The spheres (refractive index 1.59 at 589 nm) were mounted in a thin layer of gelatin between a microscope slide and a glass coverslip. A hologram, i.e. the intensity matrix $I_m$ taken with a blue laser, is shown in panel A. To obtain the intensity matrix of the light source, $I_m^{00}$, the slide was moved sideways to an area that contained only gelatin but no spheres. This reference hologram was subtracted from the hologram in panel A to obtain the contrast hologram, panel B. In panel C we show a 2-D holographic reconstruction from the original, uncorrected hologram of panel A, taken through the equatorial plane of the spheres. The image clearly resolved all spheres but also shows a
substantial noise level. Starting however, from the contrast hologram, panel B, gives a perfect reconstruction, panel D. Indeed, this image is better than a bright field image taken with the compound microscope for which diffraction rings already show up.

The power of DIH is that image information is not limited to a plane but is truly three-dimensional. 2-D holographic reconstructions can thus be performed from a single hologram at a series of selected object depths and the 3-D reconstruction of the object can be generated from such a stack of 2-D reconstructions. We have done this for the latex spheres. Panel E shows the spheres in 3-D reconstruction, viewed as if along the optical axis, that was obtained from a stack of 15 consecutive 2-D hologram reconstructions, 1 μm apart. In panel F, the same stack of 15 reconstructed sections was viewed as if along one axis of the section plane, to provide a side view of the spheres. Viewed from this direction, all spheres lie nearly in the same plane (as the sample geometry requires) and the spheres have again circular profiles. The two spheres that were in contact appear to occupy slightly different positions perpendicular to the sample plane, information that could not be obtained from conventional compound light microscopy alone. A detailed account of these studies is given elsewhere.[9]

DIH has by now been developed into a new microscopy in biology.[8]. As an example, we show reconstructed images of a unicellular marine plant cell, the diatom *Ditylum brightwellii*, mounted unstained in gelatin (Fig. 4). Images obtained using DIH (Figs. 4E, F) are compared with a bright-field transmitted-light image (Fig. 4A), a differential interference (DIC) microscopy image (Fig. 4B) using a conventional compound light microscope, and two views of a stack of images obtained by laser scanning confocal microscopy (LSCM) and reconstructed in 3-D using software (Figs. 4C, D). Note that all images are shown at the same magnification, using the same objective. Figs. 4A and 4B are sections, whereas Figs. 4C to 4F are 3-D reconstructions. It is clear that the fluorescence images of Figs. 4C and 4D, originating mostly from the cell's chlorophyll-bearing plastids, contain only a subset of the structures imaged by DIH in Figs. 4E and 4F. More complete evaluation of the DIH reconstructions can be made with reference to the original 2-D DIH images representing cuts through the cell. We refer the reader to an earlier paper where further details are given[8].

DIH can also be used successfully on macroscopic biological specimens, prepared by standard histological procedures, as for a histological section of the head of the fruit fly, *Drosophila melanogaster*. Such images reveal the structure of the pigmented compound eye, and different neuropile regions of the brain within the head cuticle including the optic neuropiles underlying the compound eye[8].

Because DIH offers a rapid and efficient approach to construct high-contrast 3-D images of a sample volume from a single hologram, a CCD camera having a fast capture rate allows us to record digitally from their successive positions the motion of particles in a sample volume, and subsequently to reconstruct images at selected depths so that the trajectory and speed of a collection of particles can be captured as 3-D data sets. To illustrate this feature of DIH, we recorded holographic images (Fig. 5A) of a live culture of the single-celled marine flagellate *Tetraselmis* (insert in Fig. 5A), contained in a 1 mm thick layer of salt water between a microscope slide and a coverslip. These algae are flattened and propel themselves by four anterior flagella. To obtain high-resolution DIH reconstruction images of the movement trajectories of the algae, we used the following procedure: i) A sequence of holograms (h) was recorded at 0.06 sec time intervals (the rate-limiting minimum interval for data transfer with our camera); ii) undesired background effects (such as the set of large concentric rings in Fig. 5A) were eliminated by subtracting consecutive hologram pairs, pixel by pixel, to generate new holograms, i.e. (h1-h2),
Holograms and reconstructed trajectories of the alga Tetraselmis in sea-water. A) Single hologram of many algae; inset: bright-field image of single alga showing flagellae. B) Sum of 10 difference holograms (from a total of 20) of the trajectories of the algae in (A). (C-D) Reconstruction of the summed hologram (B) in two planes, 350 μm apart. (Blue laser, 1 μm pinhole, source to sample distance 2.5 mm, source to CCD camera distance 20 mm.)

Fig. 5: Holograms and reconstructed trajectories of the alga Tetraselmis in sea-water. A) Single hologram of many algae; inset: bright-field image of single alga, showing flagellae. B) Sum of 10 difference holograms (from a total of 20) of the trajectories of the algae in (A). (C-D) Reconstruction of the summed hologram (B) in two planes, 350 μm apart. (Blue laser, 1 μm pinhole, source to sample distance 2.5 mm, source to CCD camera distance 20 mm.)

Acknowledgement

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References


Footnotes:

1 Members of the DIH group at Dalhousie University M.H. Jericho’, Wenbo Xu’”, and I.A. Meinertzhagen’” ‘Department of Physics and ’Neuroscience Institute
Major sudden warming and strange twist of the ozone hole over Antarctica in 2002

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The disaster of ozone depletion
The development of civilization has given rise to new problems: on the one hand, the sensitivity of humans and their economic activity to various external impacts has increased; on the other, the phenomena have appeared of human-induced disasters, whose consequences were sometimes catastrophic. In accordance with its very definition, a disaster is perceived as a sudden phenomenon (e.g. an earthquake, a volcanic eruption, etc.). However, it is everybody’s knowledge that disasters are actually the results of long-time development of relevant processes [1]. The 20th century is characteristic of the appearance of human-induced potential disasters of “slow” (or “delayed”) action, such as, for instance, the so-called “global warming” (a surface air temperature rise as a result of increased concentrations of greenhouse gases and total ozone depletion due to the emission to the atmosphere of some ozone-destroying gases (above all, freons) [2].

History and background of the ozone hole over Antarctica
It is general knowledge that the ozone layer in the stratosphere (about 90% of ozone is located in the stratospheric layer between approximately 10 and 50 km above the earth’s surface, which is called the ozone layer) protects life on the Earth from the Sun’s destructive ultraviolet (UV) radiation [2,3]. The measurements and observations of the changes in ozone come from ground-based instruments at research stations, from free-balloons, from aircrafts, and from satellites [3].

Due to the continuing human-induced destruction of the ozone layer, the UV radiation on the earth’s surface is increasing, and this in the long run may be ruinous for humans and the biosphere as a whole. In 1970, P.J. Crutzen [4] was among the first to reveal that nitrogen oxides emitted into the atmosphere as a result of using agricultural fertilizers, together with nitrogen oxides emitted by sub- and supersonic aircraft, can be ruinous for the ozone layer. In 1974 M. Molina and S. Rowland [5] revealed the ozone-destructive role of chlorofluorocarbons (CFCs) that are industrial products, used in refrigeration systems, air conditioners, aerosols, and solvents; their conclusions were later confirmed by subsequent studies. These studies won public recognition, and the authors were awarded the Nobel Prize in 1995. In September 1984, S. Chubachi [6] announced that the Antarctic station at Syowa (69°S, 40°E) had recorded a drop in ozone values during many days of the 1982 Antarctic spring and in May 1985, J. Farman et al., [7] reported the severe ozone depletion over Antarctica. It is worth noting that the USA satellite data did not record the unprecedented loss of ozone because the software processing the raw ozone data was programmed to treat very low values of ozone as bad readings [2].

In general, the “ozone hole” is defined as the area with a substantial reduction below the naturally occurring concentration of ozone in the overhead column. As a factor involved in the formation of the “ozone hole” at the high latitudes of the Southern Hemisphere, of great importance is the specific dynamics of the Antarctic atmosphere, which is characteristic of the presence of a circumpolar vortex in winter and spring seasons, which captures the circumpolar air; the air temperature then drops to -90°C, and this provokes the formation of polar stratospheric clouds (PSC). Heterogeneous chemical reactions on the surfaces of the ice particles of these clouds transform comparatively inert CINO₃ and HCl into active forms of chlorine compounds, catalyzing ozone depletion, and also combining (binding) nitrogen compounds [2].

Two types of PSC have been discovered, which consist of either particles of nitric acid trihydrate, concentrated on the nuclei of sulphate aerosols (the prevailing type), or of large particles of water ice. Both types of PSC fulfill the function of stratosphere denitriﬁcation (removal of gaseous nitrogen compounds), which is a condition necessary for the total ozone decrease. Laboratory investigations conﬁrm that the particles of nitric acid trihydrate play the key role in the formation of active chlorine compounds in the Antarctic stratosphere [2].

The discovery of the essential role of CFCs in the formation of the “ozone hole” in the Antarctic provoked interest towards studying CFCs concentrations in the Antarctic atmosphere. At first (over 20 years ago) at the Amundsen-Scott station at the South Pole, and later at the Palmer station (66.46°S; 64.04°W), regular observations of concentrations of chlorine-containing compounds in the atmosphere were performed. The data of these observations are important for the assessment of the effects of measures intended for CFCs emission reduction, in accordance

Fig. 1: The difference in the ozone and temperature vertical profiles from 2001 (cold stratosphere, low ozone) to 2002 (warm stratosphere, high ozone) (source: http://www.cmdl.noaa.gov/ozwv/ozsondes/spo/ozppp2002.html)
with the Montreal Protocol (the CFCs production was reduced by 10-20% with respect to the maximum level of the 1980s).

The exceptional event over Antarctica in September 2002

According to the September 30 Press Release from NASA and NOAA (NASA/NOAA 2002), the size of the Antarctic ozone hole was around 15 million km² during the last two weeks of September 2002, which is well below the more than 24 million km² seen in this season during the last six years [8].

Very recently, the analysis of the ozone and temperature observations showed that the most important factor for the smaller size of the Antarctic ozone hole in September 2002 was the prevalence of much higher (than normal) temperatures at the Antarctic stratosphere that resulted in limited action there of the ozone destruction processes [Fig. 1] [9,10]. The reason for the higher temperatures in Antarctica is mainly the presence of strong planetary waves (long waves that circle the globe, or planetary scale weather systems).

In addition, the basic polar vortex in the stratosphere of the southern hemisphere during 21-26/9/2002 was step-by-step elongated and distorted up to the occurrence of the polar vortex split into two cyclonic centres, leading thus to a corresponding split of the ozone hole (Fig. 2) [9,10]. This event may probably be attributed to the unprecedented occurrence of the major sudden stratospheric warming over Antarctica (induced from the strong planetary waves) [8,9].

Conventionally, sudden stratospheric warmings (increases in stratospheric temperature as much as 70°C for periods of a few weeks during midwinter) do occur in Antarctica although they are not as intense as in the Arctic [2]. However, according to the available record of observations the major warming events in the stratosphere only occur in one of two northern winters, and they do not occur in the southern hemisphere. Therefore, the most interesting thing is that the major warming of 2002 had not been seen up to now. It is worthwhile to mention here that some scientists argue that the destruction of ozone by chlorofluorocarbons is the direct and primary cause of delayed stratospheric warmings in Antarctica. If this was the major effect, the early major stratospheric warming of 2002 would not have occurred since chlorofluorocarbon loading of the stratosphere has remained relatively stable in recent years (due to the Montreal Protocol and its Amendments).

It should be emphasized however that the diminutive Antarctic ozone hole in 2002 does not support a recovery of the ozone layer, since the smaller ozone loss was mainly induced from the unexpected major stratospheric warming that occurred there.

Conclusion

The unprecedented occurrence of a major sudden stratospheric warming over Antarctica (induced from the strong planetary waves) has led to the split of the ozone hole in September 2002. These unusual events denote that there still exists a long way to go in understanding strange phenomenological twists of the Antarctic ozone hole on the long-term.

References

Opening new windows in observing the Universe

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The 2002 Nobel prizes in Physics underline the close relationship between physics and astronomy in understanding the Universe and its stellar constituents via novel detection techniques like giant underground particle detectors or space born X-ray telescopes. Raymond Davis (retired from the University of Pennsylvania) and Masatoshi Koshiba (retired from the University of Tokyo) obtained one half of the prize for discovering and detecting neutrinos from the sun or respectively from supernova explosions. The other half of the prize went to Roberto Giacconi (Director of Associated Universities Inc. in Washington) for the discovery of cosmic X-ray sources. As X-rays cannot penetrate the Earth's atmosphere, their detection was only possible via rocket or balloon flights (or later with satellites). In all three cases pioneers were honored who opened new windows in observing the Universe (www.nobel.se/physics/laureates/2002) and founded vastly expanding research fields leading to additional exciting discoveries.

Cosmic Neutrinos

Neutrinos were postulated by Pauli in 1930 as essentially massless particles without charge and with a spin 1/2, in order to permit the conservation of energy, charge and angular momentum in nuclear beta-decay \( (Z,N) \rightarrow (Z\pm 1,N\mp 1) + e^+ + \nu_e \) \( (\nu_e) \), where \( Z \) and \( N \) stand for the number of protons (\( p \)) and neutrons (\( n \)) in a nucleus, \( e^+ \) for an electron (or a positron), \( \nu_e \) for an (electron-) antineutrino and \( \nu_e \) for a neutrino. This decay mode is equivalent to neutrino (antineutrino) or electron (positron) capture when moving these particles from the right side of the reaction equation to the left in form of their antiparticles (and assuring energy/mass conservation). Antineutrinos, originating from nuclear reactors, were discovered in 1955 by Reines and Cowan via \( \bar{\nu}_e + p \rightarrow n + e^+ \), which corresponds to the reaction for \( Z=1 \) and \( N=0 \).

The Lack of Solar Neutrinos

Davis, with a Ph.D. in physical chemistry from Yale, spent almost his entire scientific life at Brookhaven National Laboratory. He specialized in radiochemical detection methods, concentrating on low level technics and background reduction. This was an excellent preparation for his plan to detect neutrinos produced in hydrogen burning deep in the solar interior from where the weakly interacting neutrinos escape (almost) freely. In the 1960s a good basic understanding of stellar evolution and solar hydrogen burning had emerged, based on the reaction cycles proposed by Bethe and von Weizäcker and many cross section measurements made at Caltech by W. Fowler's group. The pp-cycles which dominate hydrogen burning in the sun, with a net result of \( ^4H \rightarrow ^4He + 2e^+ + 2\nu_e \), produce neutrinos in four different reactions, shown in Table 1 for temperatures of roughly \( 1.5 \times 10^7 \) K.

### Table 1: Neutrino Production in Solar Hydrogen Burning

<table>
<thead>
<tr>
<th>Reaction</th>
<th>( \nu_e )-emission</th>
<th>( E_{\nu_e} ) (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( (pp) \ ^1H + ^1H \rightarrow ^2H + e^+ + \nu_e )</td>
<td>100</td>
<td>&lt;0.420</td>
</tr>
<tr>
<td>( (pep) \ ^1H + e^- + ^1H \rightarrow ^2H + \nu_e )</td>
<td>0.235</td>
<td>1.442</td>
</tr>
<tr>
<td>( ^7Be + e^- \rightarrow ^7Li + \nu_e )</td>
<td>8.017</td>
<td>0.801</td>
</tr>
<tr>
<td>( ^8B \rightarrow ^8Be^* + e^+ + \nu_e )</td>
<td>0.009</td>
<td>&lt;15.000</td>
</tr>
</tbody>
</table>

The relative \( \nu_e \)-emission rate indicates how many neutrinos are emitted relative to 100 neutrinos from the pp-reaction. Beta-decays lead to a distribution of the energy release among neutrinos and positrons, whereas electron captures release the neutrino with the total reaction energy gain. Due to the vanishingly small interaction of neutrinos with matter, it is/was extremely difficult to detect them, although \( 6 \times 10^{10} \) solar neutrinos penetrate the earth per cm² and sec. Table 2 lists a number of possible detection reactions, \( E_{\nu_e} \) is the minimum neutrino energy requirement, cc and nc stand for neutral current or charged current reactions, involving a \( Z^0 \) boson or \( W^\pm \) bosons.

### Table 1: Neutrino Detection Reactions

<table>
<thead>
<tr>
<th>Reaction</th>
<th>( E_{\nu_e} ) (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \nu_e + ^{37}Cl \rightarrow ^{37}Ar + e^- ) (cc)</td>
<td>0.814</td>
</tr>
<tr>
<td>( \nu_e + ^{71}Ga \rightarrow ^{71}Ge + e^- ) (cc)</td>
<td>0.233</td>
</tr>
<tr>
<td>( \nu + e^- \rightarrow \nu' + e^- ) (nc)</td>
<td>&gt;5.00</td>
</tr>
<tr>
<td>( \nu_e + ^2H \rightarrow ^2H + e^- ) (cc)</td>
<td>1.442</td>
</tr>
<tr>
<td>( \nu + ^3H \rightarrow ^3H + e^- ) (nc)</td>
<td>2.224</td>
</tr>
</tbody>
</table>

Raymond Davis used a tank filled with 400 000 liters of the cleaning fluid \( C_2Cl_4 \) (perchloroethylene). About one fourth of the chlorine exists as the isotope \( ^{37}Cl \), which permits to detect only neutrinos with energies exceeding 0.814 MeV, i.e. essentially only neutrinos from \( ^7Be \) and \( ^8B \) decay. The location at the Homestake Gold Mine in South Dakota, 1.5km under ground, permitted to exclude cosmic ray reactions. Radio chemistry methods allowed to extract the \( ^{37}Ar \) noble gas atoms and detect their decay with a half-life of 35 days. This experiment ran from 1967 [1,2] until 1994. On average about 0.45 decays (i.e. neutrinos) per day were detected, a result of the right order of magnitude, but only amounting to about 34% of the expected flux predicted by the "standard solar model". With this extremely precise radiochemical experiment Davis and his collaborators revealed the "solar neutrino problem" which waited for its solution about 36 years.

The Detection of Supernova Neutrinos

Masatoshi Koshiba had a background as cosmic-ray and experimental particle physicist and close connections to the University of Chicago, CERN in Geneva and DESY in Hamburg. In the Kamioka zinc mine he built the Nucleon Decay Experiment (KamiokaNDE). It was based on the detection of Cerenkov light emitted by energetic charged decay particles from nucleon decay (or e.g. energetic electrons scattered by such particles) moving with velocities larger than the speed of light in the medium water. This leads, similar to sonic booms, to radiation emitted in a narrow forward cone along the incident direction of the moving particle. The resulting light flashes can be detected with an array of photo multiplier tubes. Early versions of Grand Unified Theories (GUTs), unifying strong, weak and electromagnetic forces had predicted decay half-lives of the "stable" proton of the order \( 10^{30} \) years. The total amount of protons in 3 000 tons of water would have permitted to observe a sufficient number of decays, the non-detection provided only lower limits for the half-life. Koshiba's achievement was to adapt KamiokaNDE in 1986 to a

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Neutrino Detection Experiment based on neutrino-electron scattering $\nu + e^- \rightarrow \nu' + e^-$ (see Table 2). With improved photo-tubes it was possible to first reduce the detection threshold down to 12 MeV, later to 7 and finally to 5 MeV in the successor experiment Super-Kamiokande (also planned by Koshiba). The IMB detector in a salt mine in Ohio, built initially also for proton-decay experiments, had a detection limit as high as 20 MeV. Thus, Kamiokande was utilizalizable as a solar neutrino detector, permitting to see neutrinos from $^8$B-decay.

In 1987, on February 23rd, about three hours before the optical detection of Supernova 1987A in the Large Magellanic Cloud, Kamiokande detected a flash of 11 neutrinos with energies up to 40 MeV within about 12s [3] while IMB detected 8 neutrinos. The Cerenkov detectors could indicate the precise (collision) time, energy and incident direction of the neutrinos. In addition, all neutrino types ($\nu_e, \bar{\nu}_e, \nu_\mu, \bar{\nu}_\mu, \nu_\tau, \bar{\nu}_\tau$) were detectable, because elastic scattering of $\nu_{\mu, \tau}$ with electrons is possible via neutral currents, while beta-decay or neutrino capture (via charged currents) involves only electron neutrinos.

The energies and direction clearly pointed toward SN 1987A. This was not only the first detection of supernova neutrinos, but also the proof that massive stars experience a core collapse to nuclear densities, after passing through all nuclear burning stages (hydrogen, helium, carbon, oxygen and silicon burning) and the formation of a central Fe-core with the highest binding energy per nucleon (see Figure 1). The change of the gravitational binding energy from the size of the Fe-core to that of a neutron star of 10 km is of the order of $10^{53}$ erg. In an environment of about $10^{11}$ K neutrinos of all types are created and are the fastest escaping particles due to their minute interaction cross sections, carrying away the binding energy of the neutron star. However, for nuclear densities ($\approx 2 \times 10^{14}$ g cm$^{-3}$), these neutrinos do not leave without scattering, requiring several seconds for their escape. Within the statistics this was consistent with the observations.

Recent Developments

While the pioneers had seen the first solar and supernova neutrinos, the solar neutrino puzzle remained [4]. The European GALLEX experiment and the Russian-American Experiment SAGE, both radiochemical experiments based on $\nu_e$ capture on $^{71}$Ga, had a small detection threshold (see Table 2) and could also see neutrinos from the dominant pp-reaction for the very first time. But also these experiments detected only about 56% of the expected neutrino flux from the Standard Solar Model. Super-Kamiokande (if assuming that the detections originate from $\nu_e + e^-$ scattering, which permits a neutral and a charged-current branch) found only about 47% of the expected solar neutrino flux. The so-called atmospheric neutrino problem, related to the ratio $(\nu_\mu + \nu_\tau)/(\nu_e + \nu_\mu) = 2$ expected from cosmic ray interaction with the earth atmosphere, seemed to create another puzzle. In 2001 and 2002 a heavy water based detector in the Sudbury nickel mine in Ontario (Canada) made ground-breaking news. According to Table 2, deuterium $^2$H can undergo charged current reactions with $\nu_e$ and neutral current interactions with any type of neutrino. This led to the option to detect $\nu_e$ and any $\nu_{\mu, \tau}$ independently and showed that the sum of all neutrino events is consistent with the total number of emitted solar neutrinos. However, about 68% of the initially produced neutrinos (all $\nu_e$) were converted into $\nu_{\mu, \tau}$ [5], requiring an extension of the Standard Model of particle physics and finite (albeit small) neutrino masses. Very recent results of the KAMLAND collaboration with a new scintillation detector at the old Kamiokande site, which detects neutrinos from a number of Japanese nuclear reactors within a radius of about 100 km, are consistent and support the so-called large (mixing) angle solution [6]. Thus, there may be new Nobel prizes in the making, but in 2002 the pioneers were honored.

Cosmic X-ray Sources

Riccardo Giacconi, with a Ph.D. from the University of Milan, started out to work in cosmic ray physics. Frustrated by the low count rates he converted to a different spectral range in astrophysics, not visible before the earth atmosphere could be overcome. In 1962 X-ray astronomy was born with the start of an Aerobee rocket with three Geiger counters on board. Giacconi and his collaborators had discovered the X-ray source Scorpius X-1 and an apparently isotropic X-ray background [7]. Giacconi became the father of extrasolar X-ray astronomy by planning and building increasingly efficient X-ray satellites during his years at the Harvard-Smithsonian Center for Astrophysics. In 1970 Uhuru was the first satellite dedicated to X-ray observations. With Bruno Rossi of American Science and Engineering he developed a method to concentrate X-rays by reflecting them off paraboloid surfaces. By making use of calculations by H. Wolter (Kiel) they also achieved focusing of X-rays by a combination of paraboloid and hyperboloid segments, this permitted to build X-ray telescopes. In 1978 the Einstein X-Ray Observatory was launched [8]. The Chandra X-ray telescope, launched in 1999, was strongly based on Giacconi’s plans from 1976.
Combined with other efforts, e.g. the European X-ray satellites ROSAT, BeppoSAX and XMM-Newton, the Russian Granat and MIR-Kvant missions, and the Japanese satellites Ginga and ASCA, this led to a wealth of discoveries, related to different types of X-ray radiation from astrophysical sources. These include (i) thermal black body radiation with temperatures corresponding to X-ray energies, (ii) synchrotron radiation from electrons moving in strong magnetic fields, and (iii) X-ray line emission from excited atoms. A wealth of phenomena and objects have been observed with XMM [9].

X-ray line emission from a hot gas can be observed in supernova remnants (revealing their element composition) or in clusters of galaxies [10]. Compact objects like white dwarfs, neutron stars or black holes in binary stellar systems can accrete matter into their deep gravitational potential holes from the binary companion star, leading to a hot gas which emits thermal X-rays or in some cases also to the ignition of thermonuclear burning (type I X-ray bursts). Figure 2 shows a Chandra image of such compact X-ray sources in the galaxy NGC 4797. Mass-accreting black holes emit X-rays and in some cases jets, relativistic electrons in these jets emit synchrotron radiation. Supermassive black holes (of the order of $10^6$ solar masses) in the center of galaxies cause “active galactic nuclei”. In some cases their jets extend over millions of light years. The (initially) apparently isotropic X-ray background can now be resolved into individual sources of active galaxies with distances up to and exceeding 12 billion light years (visible with XMM and Chandra).

The study of this wealth of phenomena and objects, visible in the X-ray range, became possible after the pioneering efforts of R. Giacconi. He combines the qualities of a scientist and a manager in an excellent way, and served the astronomical community also as director of the Space Telescope Science Institute in Baltimore, director of the European Southern Observatory (ESO), and since 1999 as director of American Universities Inc. which builds together with ESO a giant telescope for cosmic infrared radiation in Chile.

References

About the authors
Gustav A. Tammann studied astronomy in Basel under W. Becker. He came in 1963 to the Mount Wilson and Palomar Observatories (now: Carnegie Observatories) to work with Allan Sandage on the expansion rate and the age of the Universe; the collaboration continues to the present day. From 1977 to 2002 he was professor of astronomy at the University of Basel. Among other honors he received in 2000 the Tomalla Prize for Gravitation and Cosmology.

Friedrich-Karl Thielemann received his PhD at the Max-Planck-Institute for Astrophysics in Garching in 1980. After having held a faculty position at Harvard University, he became professor of theoretical physics at the University of Basel in 1994. He is elected fellow of the American Physical Society and Associate Editor of Nuclear Physics A. His research interests include wide areas of nuclear physics and astrophysics.

Dirk Trautmann received his PhD at the University of Basel in 1969. After the habilitation in 1975 he spent a number of extended visits at universities in Europe, South Africa, Mexico and the US. Since 1987 he is professor for theoretical physics at the University of Basel. His research interests are related to atomic and nuclear reactions with heavy ions and cover many topics in atomic, nuclear and particle physics.
For many years, insiders have agreed, Kurt Wüthrich deserves the great prize! Both he and his group's innovations changed the field of molecular biology, and the influence on the life sciences in general is immense. Before, it was impossible to study the inner workings and the interactions of biomolecules in their natural media, in aqueous solution or within membranes. Today, we have access to more secrets of nature than ever before, and our understanding of life processes and our ability to cure diseases have grown immensely.

It seems to be common to all great innovations and achievements: The underlying idea is very simple, almost trivial; and over and over again colleagues ask themselves, why have I not had that seminal idea before? Indeed, the seminal idea of Kurt Wüthrich is very simple, and intriguing at the same time: Take two recently introduced new techniques, give them well-sounding names, combine them in an innovative, ingenious manner so that one plus one is infinitely more than two, and, finally, apply the novel methodology to a large number of highly relevant problems of great actuality. This is in a nutshell Kurt Wüthrich's secret of success. But it does not work in everybody's hands; one needs in addition his perseverance, his enthusiasm and drive, and his unbreakable belief in the ultimate success of his approach.

The two mentioned ingredients for determining biomolecular structures were two novel two-dimensional NMR techniques, COSY and NOESY, employing Kurt Wüthrich's own terminology. COSY for tracing out internuclear connectivity through chemical bonds and determining dihedral bond angles, and NOESY for measuring internuclear distances through space. And the combination of the two experiments led to his ingenious procedure for sequential assignment of the nuclear magnetic resonances of backbone protons in proteins, and later also in nucleic acids. The results became the inputs of sophisticated computer routines that, finally, calculate the best fitting three-dimensional molecular structures.

This procedure is today a standard tool, indispensable in any advanced molecular biology laboratory. During the past twenty years Kurt Wüthrich's research group solved by NMR structural questions for many proteins that could not adequately be crystallized, a prerequisite for applying x-ray crystallography.

Both techniques, COSY and NOESY, were originally invented by Jean Jeener, a brilliant Belgian physicist. In 1971, Jean Jeener proposed the very first two-dimensional correlation experiment during a lecture at an AMPERE Summer School at Basko Polje in Yugoslavia. This technique for tracing coupled nuclear spins was subsequently implemented in the author's laboratory in 1974 and introduced in 1977 into Kurt Wüthrich's research group in the hope of possible biological applications. The second experiment was suggested in 1977 again by Jean Jeener during a private discussion at a Gordon conference in Wolfeboro, New Hampshire. Its purpose was to trace networks of nuclear relaxation processes. Again, the author's research group attempted its implementation, at first for elucidating chemical exchange networks, which turned out to be easier than exploring relaxation. But soon afterwards, 1980, Anil Kumar discovered in a collaborative research project, carried out in Wüthrich's research group, that the experiment works beautifully also for cross-relaxation if only sufficiently large molecules are being used.

At this moment, Kurt Wüthrich became fully alert to the possible relevance of the two independent experiments. Their marriage was soon sealed, and their naming ceremony happened at the same time, actually to the author's dismay, being afraid of insulting the minds of purist scientists. But he soon converted also to Wüthrich's catchy nomenclature.

Although the author's collaboration with Kurt Wüthrich continued for several more years, the further seminal development happened almost entirely within Wüthrich's group. As usual, the dry spell was long from the first conception of the idea to its truly operative implementation, and it took enormous efforts, both on the experimental spectroscopic side, as well as for conceiving powerful computer data processing routines. The first protein structure, that of proteinase inhibitor Ila from bull seminal plasma, obtained entirely by two-dimensional NMR, could be published in 1985.

At this early time of two-dimensional biological NMR, there was hardly any serious competition world-wide, and never any doubt occurred that the priority for the sequential assignment of proteins and their structure determination by NMR belongs to Wüthrich's research group. But rather rapidly, other research teams acquired the necessary knowledge, and serious competition arose. Nevertheless Wüthrich's group has kept the lead up until now.

A large number of exceedingly beautiful and highly relevant biomolecular structures were determined in the mean time by his research group. Just three outstanding examples shall be mentioned: the three-dimensional structure of the complex of the peptide cyclosporin and the protein cyclophilin, of importance for the suppression of the immune response during organ transplantations; the geometry of the DNA complex of the Antennapedia homeodomain, a transcription factor from the organism Drosophila menagaster; and the structures of the mouse, bovine, and human prion proteins, of major significance for understanding the inherent processes involved in BSE and CJD diseases.

Why was NMR so successful just in Zurich? First of all, certainly because Kurt Wüthrich decided 1969 to come to the ETH, invited by the Professors Hans Günthard and Robert Schwyzer, after his successful postdoctoral years in the United States where he became, for the first time, fascinated by the potential of NMR as applied to biomolecules. But in addition, NMR had already long before a very strong footing in Zurich. Hans Staub spent his postdoctoral years at Stanford in the group of the Swiss citizen, Nobel Laureate, and ETH alumnus Félix Bloch. After being appointed in 1949 as professor of physics, he established a very lively and successful group in NMR at the University of Zurich. Later, in 1961, Professor W.H. Heini Grünacher employed NMR at the physics department of ETH Zurich for seminal studies on ice. The pioneering introduction of NMR into chemistry in Zurich in 1957 can be credited to Professor Hans Günthard and especially to Hans Primas who designed innovative high-resolution NMR instrumentation. This formed the critical nucleus for the future Nobel successes at ETH Zurich, and also for the
First EPS Technology Foresight Seminar

F. Bourgeois, EPS Technology Group

The EPS and its European dimension, cross border vision, and strong national networks can be used to promote industrial interest for new technologies and cross-fertilization. To this end, the EPS Technology Group is launching a series of EPS Technology Foresight seminars to be organized as part of renowned industrial exhibitions and conferences. These seminars will present and explain in simple terms new advances in physics, which may be of relevance for industry and the market place in the few years to come.

The first seminar, entitled “Synchrotron Radiation and Free Electron Lasers, Industrial Applications and Prospects” is scheduled to take place on Tuesday 24 June in Munich in the framework of the Laser 2003 exhibition.

The outstanding high resolution and fast data collection characteristics of the X-ray beams provided by Synchrotron Radiation (SR) sources have made them essential for collecting high quality diffraction data. They have a wide range of applications including bio crystallography for drug design, real time analysis of the growth of crystals or trace element analysis on silicon wafers.

Free Electron Lasers (FEL) generate tuneable, coherent, high power sub-nanosecond radiation pulses, currently spanning from millimetre to visible, to ultraviolet and even to X-ray wavelengths. Leading experts from academia and industry will give an overview of the SR and FEL technologies and the main benefits that industry, biology and medicine might draw from their use in the years to come.

At the end of the seminar, participants will have the opportunity to talk to the speakers.

Participation to this seminar is by invitation only and free of charge. To reserve a place at the seminar, an application form is available from the EPS secretariat. A confirmation of the booking will be sent by the EPS on receipt of the completed form.

INTAS Grants

The International Association for the promotion of cooperation with scientists from the New Independent States (NIS) of the former Soviet Union launches one open call and four collaborative calls with up to Euro 25.2 million available for international scientific research. The call deadline is 13 June 2003.

INTAS has also announced a call Young NIS Scientist Fellowships (Euro 2.5 million) and its call for Innovation Grants 2003 (Euro 500,000), each with a deadline for submission of 11 July 2003.

An information package consisting of the General Rules and a Technical Guide on the electronic submission for each of the actions can be obtained via: http://www.intas.be Section "Funding Opportunities".

2D NMR, COSY and NOESY

Two-dimensional (2D) NMR techniques generate two-dimensional maps that correlate NMR frequencies that are related. In a COSY map (red map in figure), cross-peaks arise when two nuclear spins belong to hydrogen atoms two or three bonds apart. In a protein, such hydrogen atoms belong to the same amino acid residue, as shown in the figure. In a NOESY map (yellow map in figure), cross-peaks arise when two nuclear spins are near together in space, such as the spins of Hα and Hβ in adjacent amino acid residues. The combination of a COSY and a NOESY map permits a full sequential assignment of all backbone Hα and Hβ resonances. 2D NMR spectra are obtained by specific radio frequency pulse sequences and a 2D Fourier transformation of the obtained data set. A two-pulse sequence leads to a COSY map, while NOESY maps require a three-pulse sequence. The COSY correlation is established by a quantum mechanical through-bond interaction, the so-called J coupling. The NOESY correlation, on the other hand, relies on the internuclear magnetic dipolar interaction.

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noticeboard

Elections to the Board of SNP Division

The Board of the EPS Statistical and Nonlinear Physics Division is organizing elections to replace outgoing members. Six vacancies are announced herewith. The present SNP Board announces the nomination of six candidates: Nominations have been received for M. Ausloos (and T. Tel (Eotvos University), S. Fauve (Paris), D. Sherrington (Oxford), A. Vulpiani (Rome) and D. Weaire (Dublin). Other nominations must contain a short C.V. and a statement from the candidate, and should be addressed to M. Lazar, Nador Utca 7, H 1051, Budapest, Hungary. The deadline of nominations is 15 April 2003. EPS SNP members will be informed of the resulting list of candidates and invited to vote, if necessary by the deadline of 15 May 2003. Newly elected members of the Board will be notified of the result of the election in writing by 1 June 2003.

PIXE 2004

The tenth International Conference on Particle-induced X-ray Emission and its Analytical Applications (PIXE 2004) will be held in Ljubljana, Slovenia, 4-8, 2004. The Conference topics include basic physical principles behind PIKE (physics of inner shell processes, ion beam stopping, background contributions), experimental aspects, applications of PIKE in other sciences, and PIKE in relation to other analytical techniques. The conference program will offer overview, invited and contributed oral presentations and poster sections. An equipment exhibition will be held during the meeting. The conference will be followed by the workshop "Archeaometry with IBA and related methods." For further details on the conference, please inspect the web pages: http://pixe2004.ijs.si

Nominations for HEPP Prizes

The EPS HEPP Board is calling for nominations for its

- Young Physicist Prize
- Gribov medal
- Outreach prize

Information on these prizes can be found on the HEPP Board web site http://eps-heppweb.cern.ch/eps-hepp/prizes.html together with the list of the former prize winners. The prizes of this year will be given at the International Europhysics Conference on High Energy Physics 17.-23.7.2003 in Aachen. Nominations for the Young Physicist prize, Gribov medal should be sent to Michel Spiro (spiro@hep.saclay.cea.fr, CEA-SACLAY, DAPNIA, F-91191 GIF-SUR-YVETTE CEDEX) before April 15th 2003, and nominations for the Outreach Prize to Jorma Tuominiemi (Jorma.Tuominiemi@cern.ch) before April 15th 2003.

Plasma Physics Division Elections

The PPD is organising elections for six new members in the following categories: two vacancies for magnetic confinement; two for beam- and laser plasmas, ICF; one for dusty and low temperature plasmas; and one for astrophysical plasmas and others. The term of office is 4 years, from mid-2004 through mid-2008. The present Board members are:

Elected members:
R. Bartiromo (Italy), R. Bingham (UK), C. Hidalgo (Spain), S. Jacquemot (France), J. Lister (Switzerland, chairman from mid-2004 on), J. Ongena (Belgium), M. Tendler *(Sweden), J. Stockel *(Czech Republic), F. Wagner *(Germany, chairman up to mid-2004)
* outgoing members, not eligible for re-election

The statutes of the division can be found at: http://www.eps.org/divisions/plasmaphysics.html.

Newly elected members of the Board will be notified of the result of the election in writing by 1 June 2003.

The following candidates have been nominated so far:

Magnetic confinement:
H. Bindslev (Denmark), D. Borba (Portugal), D. Campbell (Germany), T. Donné (Netherlands), V. Gusev (Russia), P. Helander (UO), B. Lloyd (UK), A. Melnikov (Russia), P. Monier-Garbet (UK), J. Noterdaeme (Germany), P. Pavlo (Czech Rep.), K. Rantamäki (Finland), W. Suttrop (Germany), P. Thomas (France), S. Zoletnik (Hungary)

Beam- and laser plasmas; ICF:
S. Atzeni (Italy), D. Batani (Italy), K. Krushelnick (UK), B. Sharkov (Russia), J. Wolowski (Poland)

Dusty and low temperature plasmas:
M. Cercek (Slovenia), G. Conway (Germany), J. Winter (Germany)

Astrophysical plasmas and others:
P. Browning (UK), E. Rachlew (Sweden), P. Shukla (Germany)

Further nominations are welcome by Individual Ordinary Members and by members of the Plasma Physics Division. Nominations must have the support of three members of the Division. Nominations must include a statement of willingness to serve on the Board for the specified time in the frame of the Division statutes and rules and must contain the plasma area in which the candidate works and his e-mail address. In order to have a large representation of EPS member states and plasma physics topics, nominations will only be accepted if there is not already a Board member of the same affiliation and if the field is not already represented by a Board member from the same country. Nominations should be sent to anne.eggeling@ipp.mpg.de. Nominations must be received no later than March 31st 2003.

The elections will be carried out from April 15th to May 15th via the internet: http://www.fusion.ciemat.es/EPVote/. The election webpage will be open from April 15th to May 15th. The elections will be announced by PLASMA-NET and the members of the division will be informed by e-mail.
Physics: Strategic issues for Europe

Martin C.E. Huber, President elect

At the outset of the 21st century, the role of physics in our society is by and large ignored. In fact, we witness widespread disinterest not only in physics but also in natural science, in general. As a consequence, learning and understanding physics is neglected and, moreover, general disinterest, reaching even the political level has led to brain drain in some parts of Europe.

Yet nearly everybody in our society makes blissful use of conveniences that have their roots in physics research. As a matter of course, people take advantage of convenient communication and transport and benefit from tools for medical diagnostics. On the other hand, most of them have no idea what is behind these conveniences—and thus also may become easy prey to shamans of fears and doom.

Little note is taken either of the momentous contributions that physics and physical apparatus have made towards a deeper understanding of our origins: the origin, structure and evolution of our world, including the Earth and life on it.

In some European countries the number of physics students has reached a dangerously low level; there, physics students aren't even numerous enough to replace today's physics teachers when they retire. How should a young person be properly introduced to physics, if there are no teachers to carry the torch of enthusiasm to pupils at an age where they are most susceptible to either take a liking to, and interest in physics or an aversion to physics? A shortage of physics teachers puts the future of our discipline in jeopardy. And, naturally, this is of great concern to EPS.

EPS is involved in trying to reverse this trend: together with the European Commission and EIROforum [1], EPS is helping to produce a European event for physics teachers from all over Europe: 'Physics on Stage'. This event will take place for the third time during this year's European Science and Technology Week, from 8–15 November. POS–3, to be held at ESTEC[2], will be the finale of 23 preceding events, where the participants in the European 'Physics on Stage' will be determined in competitions at the national level.

More needs to be done, though, and the EPS will have to be creative in this respect. The writer is planning to convene the Executive Committee (EC) for a 'journée de réflexion' on the occasion of the July 2003 EC meeting. The agenda will include, among other topics of EPS strategy, the question of how EPS can give more support to attracting students to physics.

The aim of attracting students to physics will, of course, also be advanced through the World Year of Physics 2005. The WYP, an initiative by EPS President Martial Ducloy, has been endorsed by the International Union of Pure and Applied Physics (IUPAP); and encouragement to organise local events, is being spread to physicists the world over by an International Steering Committee of WYP2005, whose members represent physical societies on all continents.

EPS will contribute to the World Year of Physics, by holding EPS–13, the next General Meeting, in Bern from 11 to 15 July 2005. This Meeting, being part of the centennial celebration of Albert Einstein's annus mirabilis 1905, will undoubtedly become one of the high points of WYP2005. The usual format of General Meetings will be changed in order to attract more physicists. A day-long 'happening' on the subject 'Physics and Society', open to the wide public, will also be part of EPS–13.

Besides these goals designed to face the problems of the future, EPS must also pursue its current strategy: EPS must continue to build strength through its Divisions and must continue to provide services to the community through its secretariat in Mulhouse. It is necessary as well to strengthen the financial base of EPS. Various means are envisaged: making use of opportunities offered by the European Commission, a drive to attract more associate members, and, yes, more Individual Ordinary Members, are a worthy goal as well.

As far as the field of physics is concerned, all physicists, whether they work in Industry or in Universities or research institutes, in applied or basic research or development, continue to face exciting challenges. The spread of physics-based instrumentation in all fields of science is bound to increase. And: is it outlandish to speculate that the situation today is similar to that at the beginning of the 20th century, where quantum physics and relativity were emerging and subsequently caused a scientific revolution? With dark matter and dark energy, two formidable problems are now in front of the community. Resolving these enigmas might again lead to a revolution in the science of the 21st century. We are testing existing physical models and theories to higher and higher accuracy and this is bound to bring a breakthrough requiring new physics.

Physics will also play a prominent role in our attempts to answer the great questions of the origin and basis of life, and in trying to understand consciousness. The question is: can we communicate an optimistic outlook to the population and decision makers? Our best bet is to do this together with young people. They are our future!

References
[1] EIROforum is a collaboration between the European Intergovernmental Research Organisations: CERN, EFDA, EMBL, ESA, ESO, ESRF and ILL.
[2] ESAs European Space Research and Technology Centre in Noordwijk/NL.
BOOK REVIEWS

Radiation at home, outdoors and in the workplace


Have you ever been asking about potential health effects from mobile phones or nuclear power plants – to state only two examples in a world where the fast developing technology influences our daily life more and more?

Radiation has always been an intrinsic factor governing life on Earth, its importance being further increased by the scientific progress of our society. For research as well as political decision making it is fundamental to acquire a profound and objective knowledge of the basics of radiation physics, leading to a deeper understanding of the radiobiological impacts on the human organism and a responsible achievement of radiation protection issues.

"Radiation at Home, Outdoors and in the Workplace" chooses a rather practical, application-oriented approach for a broad readership ranging from the graduated scientist to the interested amateur. The book covers both ionising and non-ionising radiation. In accordance with recent recommendations of the regulating authorities, the term 'non-ionising radiation' comprises not only lasers, radio- and microwaves, low frequency fields, infrared, visible and ultraviolet light, but also sound and noise. A concise picture of natural and man-made sources is drawn, which seems of particular significance in a time of repeated vehement discussions about possible biological hazards from nuclear industry, telecommunication installations and other technological achievements.

Some highlights shall be presented representatively: The effects and consequences of medical treatment facilities, e.g. radiation therapy, nuclear medicine and magnetic resonance imaging, are explained. The increased exposure both from ionising and UV radiation during air flight might obtain even more importance for human travel activities in the near future, since the development of supersonic jet aircraft cruising at altitudes of about 20 km seems only a question of time. A major part of the book is devoted to potential health risks from inhalation of the radioactive noble gas radon, formed mainly as a decay product of natural uranium which is contained in traces in building materials. With significant geographical variations, radon-related doses account on average for roughly half of the radiation exposure of the European population.

The probably strongest reason why this book not just adds to a long list of publications on this topic is the presentation of up-to-date scientific data and the inclusion of rules and regulations which have become part of the European Union legislation. However, still a wish may be expressed: Since physicists will be the main readership, a chapter outlining the construction of a human cell would further increase the quality of an otherwise highly recommendable book.

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Martin Peter 1928–2002

Oystein Fischer, René Flükiger, Bernard Giovannini, Jérôme Sierro, Jean-Marc Triscone

Martin Peter passed away suddenly on July 25, 2002. This happened the way he would have preferred, rapidly and amidst his own.

"Physics is like an aeroplane. If it stops, it falls down". Having just been appointed as a professor of physics, Martin Peter liked to repeat this sentence to his close collaborators when he founded his research group at the University of Geneva in 1962. This sentence summarises equally well his whole career: an unbounded activity and an impressive number of projects taking essential initiatives, often in a direction that nobody expected. Until he left us last July, he never stopped.

Martin Peter was a brilliant student at the Swiss Institute of Technology in Zürich, where he received the Kern medal at the end of his studies in 1952. He then decided to try his chances on the other side of the Atlantic Ocean, where he completed his thesis under the guidance of professor M.V.P. Strandberg at the Massachusetts Institute of Technology. This work earned him a position at Bell Laboratories, where he actively contributed to the ongoing study of impurities in metals. His research there was at the centre of some of the important topics in condensed matter research in the sixties: the Kondo effect, the Anderson model, and the interplay of magnetism and superconductivity. The latter subject led Martin Peter, together with Vincent Jaccarino, to propose a surprising and original idea: a ferromagnet could become superconducting when submitted to a strong magnetic field! In view of the fact that ferromagnetism normally opposes superconductivity and that a magnetic field destroys superconductivity, this prediction, since then known as the Jaccarino-Peter effect, was indeed spectacular. For a long time attempts to verify this phenomenon remained without success, and it was therefore with a certain pride that we could announce in Geneva some 20 years later its experimental observation.

When Martin Peter came to Geneva, he encountered a situation where he could make use of his talents. Under his leadership, the Institute for Experimental Physics, which soon became the Department of Condensed Matter Physics, developed rapidly. Professor Peter initiated numerous new studies; his drive for innovation and new ideas was unique and this enthusiasm stimulated his young collaborators. Soon a broad portfolio of research activities developed under his guidance: magnetic resonance, transport phenomena, elastic properties, superconductivity, positron annihilation, surface physics, and band structure calculations. At the same time, he involved himself deeply in the management of the university. First as a vice-rector and then as a rector, he made essential contributions to the development of his University, all while continuing to teach and to supervise his research. He also saw very early his responsibility towards the public and to society in general. This realisation led him to approach the local industry in Geneva to establish a common colloquium, which has been for many years an important vector for collaborations between industry and the University in Geneva: CEPIG (Colloque Ecole de Physique – Industrie Genevoise). One important result of this activity was the establishment of the Group of Applied Physics (GAP) at the University again in response to the initiative of Martin Peter.

His own research in the electronic structure of metals led him early to see the importance of numerical simulations in condensed matter physics and to propose the establishment of a common institute for numerical research in French speaking Switzerland. This proposal resulted in the creation of the IRRMA (Institut Romand de Recherche Numérique en Physique des Matériaux), located at the EPFL in Lausanne. The Swiss National Science Foundation twice called upon him to chair national research programs: the national programme on microelectronics and optoelectronics (1983 – 1991), and the national programme on high temperature superconductivity (1992 – 1995).

Martin Peter also saw the importance to strengthen the European research scene. An opportunity to contribute towards this goal came about thanks to his relations with the Hewlett Packard Company. Martin Peter proposed the establishment of a European prize in Condensed Matter Physics, and this led to the Hewlett Packard Europhysics Prize, which now has become the Agilent Technologies Europhysics Prize. Martin Peter was also in other ways active in the European Physical Society: Martin Peter was elected an honorary member of the Swiss Physical Society in 1985 and of the European Physical Society in 1998.

After his retirement Martin Peter continued to work on scientific problems, in particular the solution of the Eliashberg equations for high temperature superconductors. He continued to be invited to give scientific colloquia, as well as formal and honorary speeches, at numerous occasions in universities and academies all over the world. For his many contributions to science, he has received numerous honorary distinctions among which honorary doctor degrees from the Swiss Federal Institute of Technology Lausanne (1990), the University of Chul (1993) and University of Basel (1994). He was was elected a member of the "Deutsche Akademie der Naturforscher Leopoldina" at Halle/Saale in 1981 and he received the gold medal of the "Fondation Jean Monnet" in 1992.

Beyond his rich scientific career, Martin Peter always paid great attention to human relations, at the University, in his own family where he relished his role as a grandfather, and in cultivating numerous friendships around the world. Saddened by his loss, we who knew him will keep in memory a man with a deep personality, completely involved in science and strongly concerned by the development of his university, his city, his country and science in the world.
We are looking for a strategic thinking and communicative person for the position of

**Head of Department**

**of Condensed Matter Research with Neutrons and Muons**

PSI is a multi-disciplinary research centre for the natural sciences and technology. PSI is active in research in condensed matter physics, materials science, elementary particle physics, astrophysics and the life sciences, and also in energy and the environment. The research is carried out in collaboration with universities, research laboratories and industry from around the world. The Institute is one of the leading user laboratories for the world scientific community. In this function it develops and operates complex research installations which demand exceptionally high standards of know-how, experience and professionalism. These installations include the Spallation Neutron Source, SINQ, and the facilities for Muon Spin Spectroscopy, SPS.

The Challenge

As Head of the Department for Condensed Matter Research with Neutrons and Muons, you will have scientific and technical responsibility for the exploitation and further development of the research facilities SINQ and SPS. In addition, you will supervise PSI's own research with neutron scattering and muon spin spectroscopy.

Your Profile

For this extremely demanding task we are searching for a highly qualified scientist of international standing in the fields of condensed matter or materials science, with experience in neutron scattering and/or muon spectroscopy. You will be motivated to promote collaboration with researchers at the PSI Synchrotron Light Source, SLS, and with external research groups from Switzerland and throughout the world. Proven leadership and the ability to motivate people are essential requirements.

Prof. Ralph Eichler will be happy to answer questions: Tel. +41 (0)56 310 32 16; e-mail: ralph.eichler@psi.ch.

Please send written application by 30 April 2003 to:

**PAUL SCHerrer INSTITUTE**, Human Resources, Mrs. Elke Baumann, Ref. 3000, CH-5232 Villigen PSI, Switzerland

Further job opportunities at PSI may be found at: www.psi.ch
COURSE CLIV “Physics Methods in Archaeometry” 17 – 27 June
Directors: M. Martini - Università di Milano Bicocca (Italy); M. Milazzo - Università di Milano (Italy); M. Piacentini - Università di Roma “La Sapienza” (Italy)
Contact person: A. C. FELICI - Dipartimento di Energetica, Università di Roma “La Sapienza”, Via A. Scarpa 14, 00161 Roma (Italy), Tel.: +39-06-49766322, Fax: +39-06-44240183, varenna@uniromal.it
Deadline for application: May 1st, 2003

Directors: F. Mallamace - Università di Messina (Italy); H. E. Stanley - Center for Polymer Studies, Boston University, MA (USA)
Contact person: F. MALLAMACE - Dipartimento di Fisica, Universita di Messina, Vill. S. Agata, CP 55, 98166 Messina (Italy), Tel.: ++39-090-6765016, Fax: ++39-090-395004, Francesco.Mallamace@unime.it
Deadline for application: May 1st, 2003

COURSE CLVI “Research on Physics Education” 15 – 25 July
Directors: E. F. Redish - University of Maryland, College Park MD (USA); M. Vicentini - Università di Roma “La Sapienza” (Italy)
Contact person: C. TARSITANI - Dipartimento di Fisica, Università di Roma “La Sapienza”, F. le Aldo Micro 2, 00185 Roma (Italy), Tel.: ++39-06-49913483, Fax: ++39-06-4463158, carlo.tarsitani@romal.infn.it
Deadline for application: May 15th, 2003

COURSE CLVII “The Electron Liquid Paradigm in Condensed Matter Physics” 29 July – 8 August
Directors: G. F. Giuliani - Purdue University, West Lafayette IN (USA); G. Vignale - University of Missouri-Columbia MO (USA)
Contact person: M. POLINI - Scuola Normale Superiore, Piazza dei Cavalieri 7, 56126 Pisa (Italy), Tel.: ++39-050-509038, Fax: ++39-050-563613, m.polini@sns.it
Deadline for application: May 15th, 2003

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