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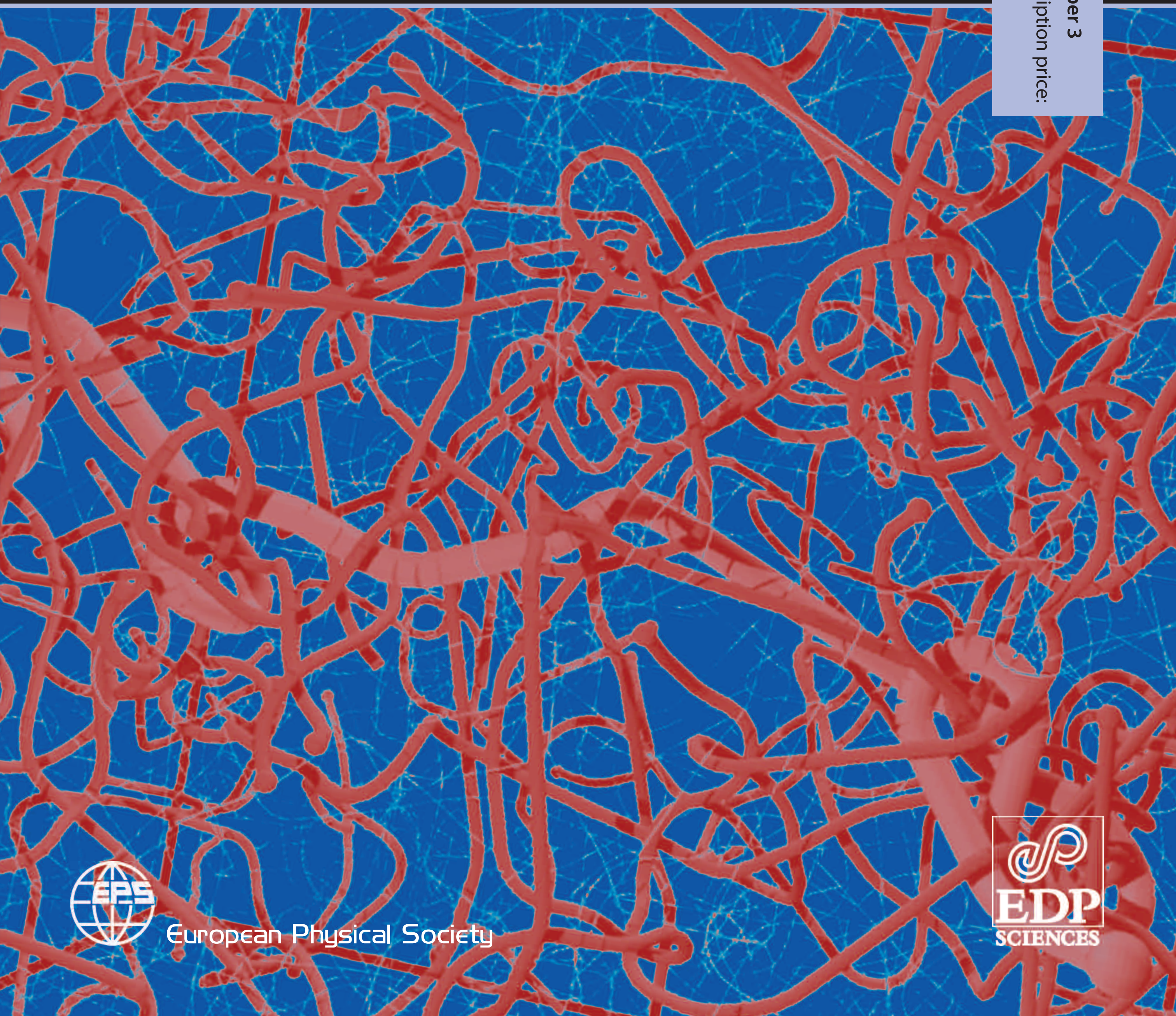
Condensed matter theory by computer simulation

Toying with physics

Fun with the setting sun

Bounded modes to the rescue of optical transmission

A thermo-magnetic wheel



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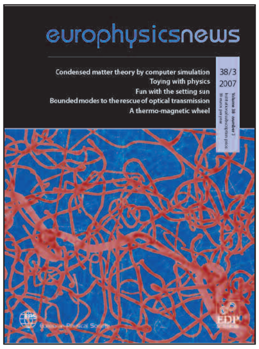

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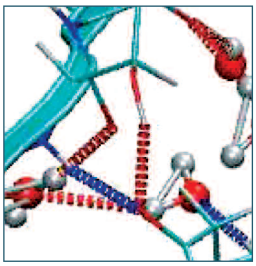
Cover picture: See Figure 2, p.21 in article "Condensed matter theory by computer simulation: from materials to chemical biology"



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My views and programme [EDITORIAL]

Volunteers are important actors in many of the activities of the European Physical Society. The motives for their engagement vary though they are often grounded in an appreciation of the physics field in which one is embedded, and from the insight that physics benefits if carried out jointly on a European scale.

In my own case it is rather obvious. The remarkable progress fusion research has made over the last decades, thanks to its European-wide organisation was a determining factor in my involvement in the Plasma Physics Division as chairman. The European dimension of plasma physics research allowed the building and operation of JET in the UK, currently the largest and most relevant fusion device, and it ultimately made Europe the best choice as the ITER site. ITER, to be built in Cadarache, France, though still a scientific device, will be the first fusion reactor, producing a factor of 10 more power than externally invested.

Another reason for my European engagement stems from my German origin. My generation was brought up with the view that the German post-war political problems would be solved by and within the European unification process and that the future would be European. The European Union that was founded exactly 50 years ago with the conclusion of the Treaty of Rome (March 1957) led to the creation of both the EEC and Euratom. The fusion programme is part of the Euratom contract. Science has profited from this integration but it has also contributed in a unique way to the evolution of a European identity: science creates values.

An exciting decade lies ahead for physics. Large and promising devices have been approved and will start operation in the near future. In this year and next, science in Europe will carry nature back to its beginnings and conditions will be created with the LHC, the Large Hadron Collider at CERN, closer than ever to those shortly after the Big Bang.

The 7th Framework Programme foresees a budget of more than 54 Bn € for research. The support of basic research with 7.5 Bn € and the creation of the European Research Council establishes a new horizon for science. The creation of the ERC will introduce an element of scientific self-organisation in the 7th Framework Programme and entrust scientists with more decision power in the support of projects and the distribution of resources for research. The implementation of the Bologna process is expected to lead to a higher mobility of students and will introduce competitive elements in attracting the best of them. The creation of the European research area will continue and, from the many steps already taken and those foreseen, it will gain further momentum.

The enthusiasm for these developments should not distract from reality. The funds made available by the European union for R&D account for only 6% of the EU overall budget for research. Many initiatives still suffer from the bureaucratic structure of distant institutions and, for sure, every effort to make administrative processes simpler will pay off. The same is true for making the application process more transparent and more predictable in order to prevent investments of time, motivation and resources by the applicant that are in vain.

Serious concerns remain about physics education in schools and its continuation in universities. I support the basic principles expressed in the EPS educational policy position paper: Bachelor education in physics should have a largely common curriculum to facilitate student mobility between universities and countries, both during and after the bachelor programme; Masters degrees need to be more varied and involve specialisation in particular areas of physics or combinations of physics with related disciplines; and Doctoral degrees should not be modularized to any large extent.

These principles also address major problems associated with the Bologna process. The Bachelor in Physics may not meet the needs of industry unless curricula are adapted. On the other hand, it may lead to a reduction in the number of PhD students and weaken the scientific base. The major concern of the EPS •••

••• as expressed in its policy statement on PhD degrees is the strong and centralised inclusion of the PhD thesis work into the goal of European harmonisation of higher education. A large fraction of research is carried out by PhD students under the guidance of their supervisors. To change the weighting in favour of more educational and less research elements in the preparation for a PhD thesis may lead to a set-back of European research. The training PhD students receive is not only a first step in an academic research career but also for a job outside academia. The practical treatment of a research problem during a PhD programme is the best preparation for both career paths.

A major goal of EPS is to contribute to the development of balanced conditions for physics in all of Europe. The consequences of the termination of the Soviet Union represented a tremendous challenge for the maintenance of this goal and principle. EPS has helped physics in the FSU countries to organise themselves under democratic governance and to establish their national roles and to develop contacts within the European research structures. This process has not yet come to an end but the trend to normalisation is evident. The EPS Group "Physics for Development" is strongly motivated to help the countries south of the Mediterranean by selected educational programmes, providing support for summer schools and by giving grants to enable contacts to be made with our research network. However, a long way is still ahead of them (and us).

A topic which deserves and requires continuous attention is to improve the chances of women in physics. The motivation may not necessarily be altruistic but may well have its origin in the recognition that physics cannot do without 50% of its talent and intellectual potential. I hope everyone will agree when I say that progress in physics needs also the perspective and insight of women and that research teams benefit from female scientists in their staff. Whenever there is a possibility, EPS should look for talented women to fill a vacancy in its own structures. Its policy must be that the Divisions and Groups welcome women onto their Boards, that women are invited to become members of conference Programme Committees and that the outcome of these organisational steps bears fruit – that more women give invited talks at conferences in recognition of their capabilities, and improve their chances to advance their careers and play a more accepted role. EPS will continue to support women in their interest to develop networks and to form and maintain organisations to promote their case. As the necessity to provide equal opportunities is also a task of national societies, better cooperation and coordination might accelerate this process toward normalisation.

EPS encourages the development of a physics publication platform made up of scientists, learned society publishers, and commercial publishers. The services sciences require from publishers of scientific journals are the maintenance of a high scientific standard by an efficient refereeing system, electronic accessibility in a form which fosters international cooperation and an interdisciplinary approach, and good functionality for documentation and retrieval. Scientists expect from publishers and journals fair treatment of their papers, quick publications both on the internet and in print, services regarding the quality and accessibility of the paper as well as on-line availability of archived papers, and a journal policy which continuously increases the impact factor and thus improves the reputation of its papers and of its contributing authors.

Papers with the highest prestige in our field are mostly published in journals based in the United States. This is partly due to the excellent research carried out by our American colleagues and friends but it is also owing to the circumstance of a homogeneous research area within the US, with publication in one language. In Europe, our long research tradition reflects the national history in science and the publication landscape is more diverse. Many national journals have published what is now to a large extent the basis of our physics inheritance. It also has to be recognized that the national physics journals of Eastern countries have played an important role after the breakdown of the Soviet Union as focal points in the phase of restructuring.

The attractiveness of APS journals would be acceptable if there were not a close link between international recognition of the journal (focused on its impact factor) and career chances of the authors. The consequence is that the system has a tendency to instability, to an increasing concentration on a few highly attractive journals. Understandably, authors tend to submit to the journal with the highest prestige. It has become a sportive element in submitting papers first to the most prestigious journal at the expense of possibly losing some time in the case of its rejection. Rejected papers are re-submitted to what develops as a second category of journals – at least in the eyes of those who decide on careers.

Dissemination of scientific results is a major task of EPS. We will, therefore, have to watch carefully the reaction and countermeasures of European science and science managers to the trend that – to a large extent - scientific achievements are not published and archived where the underlying research has been financed and the scientific results have been achieved. Fair and open competition is a fundamental principle of the Europeanisation process. The EPS is concerned with the fragmentation of the publication industry in Europe and its consequent contribution to the growing monopoly of US publications. Scientists need more choice of high quality publications. Europe's publishers should therefore be supported to improve the attractiveness of their journals. The foundation of an umbrella organisation of European based publishers would help and ease the dialogue between publisher and the national or EU-wide representation of physics research. Scientists, on the other hand, should contemplate the mechanisms which cause the publication market to concentrate and whether this – in the long run - is in their true interest. Close cooperation between scientific community and regional publishers is necessary to avoid a loss of diversity with consequences that are difficult to foresee. EPS will carry out a major campaign in 2007 to enhance the visibility and attractiveness of European journals in general, with a specific focus on EPL.

Each president has to formulate "his (or her)" programme for his (or her) two-year term. As presidents come and go it is mandatory to respect continuity e.g. in the topics mentioned above. Of particular importance to me is that the Divisions and Groups are encouraged and supported to carry out the tasks of their mandates, predominantly the organisation of conferences and the dissemination of scientific results. EPS should continue to offer the most relevant conferences in the respective fields and to make the good ones even better. The scientific material presented in these conferences is of high value and should not be lost. In many cases the conference organisers take care that the material is published as refereed papers. Where this is not the case appropriate forms of publication and archiving have to be found. Close collaboration with the EPS Secretariat is offered. The electronic means of communication and exchange will continuously be improved. The work of the Divisions should also receive a higher awareness in Executive Committee and Council and the Divisions should be better integrated into the overall development of EPS. A forum has been initiated where the Divisions and Groups of EPS can communicate with each other and where exchange with other EPS structures is possible.

Another element I am interested in is to intensify the cooperation with the National Societies. Although national support will continue to be their major financial source, research and development will increasingly be shaped by the European Commission and its organisations. To make best use of this development, we should aim at closer cooperation between National Physical Societies and EPS. The agenda for the Council meeting should therefore provide room also for joint strategic discussions. We have to follow the political developments , the social trends of the EU on aspects of physics education and research, to exchange the necessary information and to analyse it as a community. We should also seek an understanding of the broad spectrum of responses within the largely different national societies.

This exchange of views and the joint planning should be at all levels of the EPS:

- The Council should promote exchange of information between the national societies. EPS and national physical societies should identify joint projects. The Council should be used to define structures and distribute tasks to tackle and solve them. An example would be the continuous analysis of the impact of a homogeneous bachelor/master education in physics. In order to make this tremendous task possible, it might be sufficient that each national society identifies one or two physics departments where the information is provided, exchanged and analysed. Thus, we may obtain an early view on this development before the large and official studies appear, that will hardly single out and reflect the specific issues of physics. •••

Curiculum Vitae

Scientific CV

I studied physics at the Technical University in Munich (TUM) and I got my PhD degree in 1972. This period at the TUM was exciting because a new physics department was founded with young professors, many returning from the States. My field was low-temperature physics, studying rotating superfluid He and the question whether the surface excitations of HeII were quantised like those (rotons) of the bulk (they are not). As a post-doc at Ohio-State University, I expanded to superconducting metals studying the questions whether conduction electrons contribute to the heat transfer from metals to Helium (Kaptiza resistance). Having experienced the first energy crisis in the USA, I happily accepted an offer of the Max-Planck-Institute for Plasma Physics (IPP) in Garching/Munich. It implied a jump in temperature scale from K to eV (plasma notation). I started as a diagnostician on the Pulsator tokamak and continued on the ASDEX tokamak being in charge of the physics of neutral beam heated plasmas. Into this period fell the discovery of the H-mode (the H-mode is a dynamic state of the plasma with the interesting feature that stronger thermal forces lead to lower turbulent fluxes; the transition into this regime happens in a self-organised form. The plasma in the H-mode is closer to the programmatic goals of fusion). In 1987, I worked with the Princeton team on their TFTR tokamak. After 15 years of tokamak research, I felt it was time to change and I took over the leadership of the experimental stellarator programme of my institute. Now, I am more than 15 years in this field.

The physics of high-temperature fusion plasmas has many interesting and relevant features – aspects of magnetic field geometry, equilibrium, stability, collisional and turbulent transport, plasma wall interaction, heating and diagnostics. During a long professional life in this field (I was born in 1943), one gets in touch with all issues because plasmas are complex and involved, highly non-linear systems. My main interest is, however, plasma confinement.

Career CV

I had a teaching assignment at the Ruprecht-Karls University in Heidelberg, was honorary professor at the TUM and I am at present full professor at the Ernst-Moritz-Arndt University in Greifswald.

In 1988, I was nominated Fellow of the Max-Planck-Society and Director at IPP. I was project head of ASDEX tokamak, W7-AS stellarator and for 2 1/2 years of the Wendelstein 7-X stellarator project to be built in the new MPG institute in Greifswald right at the Baltic See. I am head of the experimental department E3 since my nomination, served for 12 years in the Directorium of IPP and was spokesperson of the Greifswald branch for 8 years.

- The divisions and groups should form closer cooperation with their national counterparts, wherever such structures exist. EPS divisional conferences often cooperate with the local institutions in the organisation of conferences. This element of cooperation and agreement should represent a natural part of the EPS culture. Whenever a divisional Board meets in an EPS member country, an exchange with representatives of the national science field should become an agenda item as a matter of course.
- Those who play a specific role in the societies (EPS and national), because they deal with administrative or legislative issues or they guarantee the societies' continuity, have a specific and general responsibility to develop their own perspective. They should also create forms of exchange and cooperation.

Another topic I am concerned with is energy (actually, the concern of many). Europe has a need for the availability and accessibility of a reliable flow of energy to maintain the productivity and competitiveness of its economy and the equilibrium of its societies. Europe's own energy sources are running out and it relies increasingly on imports at a time when for the first time prices of the raw materials are set by market laws. The increase in gasoline prices provides us with a daily bulletin on the growing scarcity of this commodity.

One way of looking at the EPS is that we represent the knowledge of 100000 physicists. Physics is playing a major role in the energy issue through the development of fission energy, in providing nuclear data for alternative processes, in the development of new concepts such as accelerator-driven sub-critical reactors, and in the storage, reprocessing and transmutation of waste. Physics also plays an obvious role in the development of fusion energy in the form of magnetic confinement or of inertial fusion. But physics is also of high importance in the techniques of renewable energy and in energy-saving technology. Photovoltaic electricity production is still a rich research field with many unexplored possibilities using new materials, plastic substances, material combinations or the integration of nano-technologies. Exciting discoveries and technological breakthroughs can be expected in this area. Similar arguments on the importance of physics apply to the development of fuel cells and of techniques to store energy - specifically electricity.

Energy is the topic of the EPS Technology Group (TG). In addition, energy is one of the topics of the Nuclear Physics and the Plasma Physics Divisions. It plays a role in the Condensed Matter Physics Division (photovoltaic processes, materials, etc.) and in the Quantum Electronic Division (light sources). The Physics in Life-Sciences Division is the bridge to biotechnologies. The Environmental Division is knowledgeable on the atomic and molecular physical-chemical processes in the atmosphere and deals thus with the environmental consequences of energy conversion. These different activities will be jointly discussed within a newly founded Energy Working Group of the TG. The work will concentrate on science and technology not on political or social aspects. We should demonstrate, however, that physics is not synonymous with nuclear energy only; our goal should be the development of CO_2-free electricity production and, in the long run, of a hydrogen-based transport system.

Environment and global warming are considered to be supra-national topics. This is not the case, however, with energy where the debate is mostly restricted to the national needs, opportunities and interests. This is not an appropriate association because energy is the primary and environment the secondary problem. A global secondary problem can hardly be solved by a local approach to the primary problem. Europe still lacks a joint energy policy; solutions are sought nation-wide and the strategies are widely different. Efforts are underway to change this. Physics should be ready both nationally and EU - wide when this issue is and remains of front-page concern. I would suggest that the national physical societies form energy working groups, if this is not yet done. We recently had a meeting of the

existing groups (Denmark, DPG, Finland, Hungary, IOP, Lithuania, SFP, and Sweden) and we realised that EU-wide cooperation is necessary and timely.

Let me summarize: I would wish to continue the efforts of past Presidents to make the EPS more effective and to achieve a better balance within EPS between East-West, North-South, male and female physicists, physics and society, and smaller and larger physical societies. I should also wish for EPS to continue its care for its members, its involvement in physics education, and its efforts to maintain a diversified publication scene. Last but not least, I would wish that EPS should continue its presence in the European science policy sphere, with its goal - the promotion of the case for physics. All this must be carried out in a transparent and comprehensible way, governed by the ethical principles of science.

How to do all this? This brings me back to where I started - the role of the volunteers, those who make a donation to the society, not in money but, of more value, in their time. We must cooperate in a creative atmosphere; ideas have to be treated like a gift and the maintenance of motivation is the uppermost imperative. We do not cooperate under an employment contract but under a social contract - to make the best use of the investment of our own time and that of others. ■

Friedrich Wagner, EPS President

Laudation Ove Poulsen

at the occasion of the end of his EPS presidency by the new president, F. Wagner

Dear Ove,

one president comes, another one goes. I want to thank you, Ove, on behalf of the members of the Executive Committee, the Secretariat in Mulhouse and of all of us who are assembled here, thank you for your leadership and your contributions to EPS. I am sure, everyone in this room will have the desire to shake your hand later and thank you personally.

I will not be able to reflect all initiatives you took and honour all of them. You picked up many important issues, initiated many important and urgent steps with the consequence that I found it difficult for me to identify additional urgent issues to further shape and expand and complement the portfolio of EPS activities.

You put education and the publication issue onto the table and on the agenda; you considered the general issue of physics and society and you organised or participated or represented EPS in many important meetings. You were fully aware of what EPS should do and could manage and you developed your concept and followed it through. This may have to do with your Danish inheritance, decide where to go and then strictly follow the course. Nevertheless, you presented your suggestions, had them discussed, allowed others to influence them, and then a decision was taken. You represented EPS as an open, constructive and determined personality. I am happy for my own presidency to have you still on board.

You probably all followed this national competition last year – no I do not mean the soccer championship but something much more exciting, the selection of the happiest people on earth and – low and behold – the happiest people are the Danes. This happiness index will now further increase, because one of the Danes, Ove Poulsen, will get a present now and this is always a source of happiness.

An important issue for you, Ove, was always to reach, what you called, the forward looking dimension. You educated and trained individuals and committees to eventually stop talking about the past and finally come to and start to adopt the forward looking dimension. But, you yourself also took the necessary steps in the right direction. We physicists are trained to and have the natural desire to do everything under quantified conditions. In order to quantify, in the future, the necessary steps when the stage of the forward looking dimension has been reached, you can use now this present - David actually had the idea. It is a step counter, a pedograph, it is also called an odograph, not an ovegraph – but phonetically rather close. From now on, the forward looking dimension has a scale. (Maybe, we have a picture of the device to add or a photo when I handed it over)

You get also a present from me. As you know, I very much honour everything around Max Planck. Here is his book the "Philosophy of Physics". I found it in an antique shop in Florida – a good sign for those who retire, but this is not the issue here. It fits to the memorable moment here to quote a few sentences from this book because they deal with supranational aspect of physics and fit to EPS and they address the relation between physics and ethics, an element of our field where you are strongly engaged yourself:

"If science is unable or unwilling to extend beyond the limits of the nation it is unworthy of the name of science; and in this connection physics enjoys an advantage over other branches of science. Nobody will dispute that the law of nature are the same in every country; so that physics I not compelled to establish its international validity (…). Ethics also is supranational, otherwise ethical relations could not exist between the members of different nations. Here again physics takes up a strong position. Scientifically it is based on the principles that it must contain no contradiction, which is terms of ethics implies honesty and truthfulness; and these qualities are valid for all civilised nations and for all time; so that this scientific principle may claim to rank among the first and most important of virtues." ■

Denis Jérome, Editor-in-Chief of EPL during an Eventful Time [PUBLICATION]

The retirement of Denis Jérome as Editor-in-Chief of Europhysics Letters, at the end of his three-year term, is an excellent occasion to recall his great merits in advancing this journal. EPL - and physics in general - have greatly benefitted from the scientific leadership he brought to this foremost letters journal published in Europe.

Denis Jérome's actions as Editor-in-Chief, all based on his scientific stature and experience from earlier editorial functions with the Journal de Physique and the European Physical Journal-B, have been invaluable for bringing EPL closer to the aim of becoming a letters journal exploring the frontiers of physics that is recognised not only in Europe, but worldwide. In tune with this development, and to steer clear of being viewed as journal with an exclusively European outlook, the Board of Directors of EPL has now introduced the new designation 'EPL' rather than the explicit 'Europhysics Letters'.

Denis Jérome's research activities are devoted to organic conductors. His discovery, in the early 1980s, of superconductivity in some organic materials was an event with worldwide impact on condensed-matter physics. In 1985 he was given the Holweck Prize, an honour awarded annually, alternately to a British physicist by the French Physical Society and to a French physicist by the U.K.'s Institute of Physics. Moreover, Denis was elected, during his term as Editor-in-Chief of EPL, as a member of the highly selective French Academy of Sciences.

During his tenure, Denis Jérome succeeded, as part of the regular renewal of the Editorial Board, in persuading many leading scientists to collaborate as Co-editors, at the same time keeping in mind both an appropriate coverage of fields and an adequate balance of nationalities.

Besides this great effort and the ever-present, daily duties of an Editor-in-Chief, Denis had also to face two major transitions in the operations of EPL. The Editorial Office was moved from the former location of the EPS Secretariat in Petit-Lancy to the new headquarters of EPS in Mulhouse. As part of this move, a younger team under Yoanne Sobieski replaced the well-trained former team under Staff Editor Edit Thomas. In a new Production Contract for EPL, the Institute of Physics Publishing (IOPP) joined the previous partners EPS, the French Edition Diffusion Presse Sciences (EDP Sciences) and the Società di Fisica Italiana (SIF), and thus strengthened the journal. Throughout all these changes, Denis Jérome has been a very active participant and trusted consultant.

EPS, as the learned society responsible for the scientific quality of EPL, as well as all the owners of EPL [1], have many reasons to be grateful to Denis Jérome for his outstanding stewardship of EPL over the past three years. ■

Martin C.E. Huber and Claude Sébenne

[1] The Owners of EPL are the four Category-A Members, the European Physical Society, the French Physical Society, the Italian Physical Society, and the Institute of Physics (UK); and the nine Category-B Members: the Austrian Physical Society, the German Physical Society, the Hungarian Physical Society, the Institute "Ruder Boskovic", the Netherlands Physical Society, the Portuguese Physical Society, the Pool of Scandinavian Physical Societies (namely the Danish, Finnish, Icelandic, Norwegian and the Swedish Physical Societies), the Swiss Physical Society, and the Turkish Physical Society; as well as two Associate Members (the Institute "Josef Stefan" and the Spanish Royal Society of Physics).

ASSE 2006 (Advanced School on Space Environment) [CONFERENCE REPORT]

From the 10th to the 16th of September 2006, an Advanced School on Space Environment (ASSE2006) was organized jointly by Consorzio Area di Ricerca in Astrogeofisica – CARA, International School of Space Science – ISSS (www.cifs-isss.org) and World Institute for Space Environment Research – WISER (www.cea.inpe.br/wiser). The school was held at the Scuola Superiore G. Reiss Romoli (SSGRR), an excellent Hotel/School located in the medieval town of L'Aquila, 100 km east of Rome, Italy, surrounded by the beautiful mountains of the Gran Sasso d'Italia.

The main goal of the school was to provide an overall view of the main physical processes acting on the sun-earth environment treated as a unique system. This kind of approach allows a significant improvement in the global knowledge of the entire system, paying particular attention to changes on the Sun, which influence the near-Earth space and to the multiple physical processes that occur sequentially in each domain. It is a dramatic fact that our understanding of the physical phenomena that contribute to Space Weather is still too limited to allow for reliable and useful forecasting. Additional theoretical and data analysis efforts are strongly needed and young scientists are encouraged to continue in this direction. Educating students today about this kind of problem assumes a remarkable importance because of associated economical and social repercussions in the future.

Keeping this in mind, lectures were organized in such a way as to allow the young researchers attending the school to become fully aware of the interdisciplinary nature of this subject; moreover, their attention was addressed to the improvements and progress which are needed for a better understanding of the Sun-Earth domain as a whole, and to the critical aspects of Space Weather. Thus, lectures ranged from the solar interior to the solar atmosphere, to interplanetary space, magnetosphere, ionosphere, geomagnetic storms and substorms. Moreover, the programme also •••

Prof. V. Dose, new Editor in Chief of EPL [LAUDATION]

Professor Volker Dose, an active member of the physics community for 40 years, has been appointed Editor-in-Chief of Europhysics Letters (EPL; www.epljournal.org). Professor Dose will take on the role of Editor-in-Chief from Professor Denis Jérome (Université Paris-Sud, Orsay) at the next meeting of the EPL Editorial Board to take place in Paris, 11- 12 May 2007.

Following his appointment, Professor Dose said, "This is an exciting time for EPL. In 2007, the journal starts the next phase of its life: a new vision as a truly international journal at the forefront of physics, a new website, and new journal cover and format. I look forward to working with the Editorial Board and the international scientific community to grow our journal."

Professor Volker Dose took his PhD at the University of Zurich in 1967 and in 1971 was appointed Professor at the University of Würzburg. Later, he became Director and Scientific Fellow at the Max-Planck-Institute of Plasma Physics in Garching, and since 1991 has also been Full Professor at the University of Bayreuth. His research experience is diverse, including magnetism, surface and plasma physics, collisions and statistics, specifically Bayesian statistics. He has applied the method of Bayesian statistics to largely different problems, which range from X-ray astronomy to plasma physics and climate research. This breadth in his research is reflected by the citation of the **Robert-Wichard-Pohl-Prize 2005**, which Volker Dose received from the German Physical Society. It read: … for *his outstanding interdisciplinary contributions to the physics of atomic and molecular hydrogen, to the electron band structure of solid states and to the Bayesian probability theory*.

Prof. Dose was Deputy Dean of the Faculty of Physics and Astronomy of the University of Würzburg from 1976 to 1978 and again from 1982 to 1983; from 1983 to 1985, he was its Dean. From 1984 to 1986 he was Chairman of the Surface Physics Division of the German Physical Society and from 1985 to 1988 Deputy Chairman of the German Vaccum Society; from 1987 to 1998 he was Chairman of the Bavarian Section of the German Physical Society and from 1987 to 2000, V. Dose was Co-Editor of Applied Physics A.

Volker Dose`s scientific achievements are honoured by many awards. The Robert-Wichard-Pohl-Prize has already been mentioned. He has also received the Grünewald-Medal of the city of Würzburg and the Honorary Promotion Dr. rer. nat. by the Faculty of Physics of the University of Kassel. ■

••• treated basic concepts such as non-linear processes in space physics, and magnetic reconnection.

The school was organized in plenary sessions; there were 18 lecturers who gave a 80 min lecture each. Most of the invited lecturers of ASSE 2006 derived from the list of authors of the Handbook of Solar-Terrestrial Environment edited by Y. Kamide and A. C.-L. Chian, to be published by Springer in 2007. About 40 students with graduate and undergraduate background from 10 different countries attended the school; they were also given the possibility to present their research activity during the oral and poster sessions dedicated to them throughout the week. The directors of the course were: R. Bruno (IFSI-INAF, Rome, Italy), U. Villante (University of L'Aquila, Italy), A. Chian (INPE, Saõ José dos Campos, Brasil), Y. Kamide (STELAB, Nagoya University, Japan). ■

Roberto Bruno (Rome)

▶ Group picture of the attendees of ASSE2006 school. Moving from left to right, arrows indicate the directors of the school: Y. Kamide, U. Villante, R. Bruno and A. Chian.

Ioan Ursu 1928 – 2007 [OBITUARY]

Alexandru Calboreanu,
President Romanian Physical Society

Ioan URSU, the fourth President of the European Physical Society, has passed away. He suffered a fatal heart attack on April 17 2007, aged 79.

The academic community will remember Professor Ursu for his contributions to physics, as a professor and researcher in Cluj and Bucharest, as the Director of the Institute of Atomic Physics in Bucharest from 1969 to 1977, as the President of the National Committee for Nuclear Energy from 1969 to 1977, as the Prime Vice President of the National Council for Science and Technology and a member of the Romanian Academy of Sciences. He has also had an outstanding international profile.

Born in the Transylvanian village Manastireni, he began his studies in nearby Cluj-Napoca. During the Second World War, he attended high school in Turda, as Cluj had been ceded to Hungary, following the Vienna dictate. After the war he graduated from the Faculty of Physics and Mathematics at Babes-Bolyai University in Cluj, where he obtained his doctorate in 1956 and Doctor Habilus in 1967. He had a successful career in Cluj beginning as a laboratory demonstrator (preparator), and ending as dean of the physics faculty and Vice-Rector of the University. In a private discussion he praised with modesty many of his university mentors and colleagues, Augustin Maior, Aurel Ionescu, Ion Dragan, Victor Mercea and Aurel Novacu.

In Cluj Professor Ursu became interested with what would prove to be one of the great atomic physics ideas – electronic paramagnetic resonance. This led to a fruitful international collaboration which brought him in contact with two exceptional personalities: Freeman Dyson and Serg Turkevich. Two books published in 1959 and 1965 have become textbooks for generations of students. A grandiose volume, "La résonance Paramagnétique Electronique", published by Dunod-Paris, also appeared in 1968. In its introductory presentation Nobel laureate Alfred Kastler declares "Le Professeur Ioan Ursu de l'Université de Cluj (Roumanie), est un expert internationalement connu dans le domaine de la résonance paramagnétique électronique". In the Russian translation another Nobel laureate A.N. Prokhorov, expressed similar appreciation. Further working visits in Germany, the United Kingdom, Switzerland, Italy, Russia, increased his reputation and recognition in the scientific world. In Romania he created the school of scientists that in Bucharest, Cluj and Iassy continue successful research in electronic and nuclear resonance.

His reputation led to his nomination as Director of the Institute of Atomic Physics in 1969, twenty years after it was founded by Horia Hulubei. He also assumed important state positions such as the presidency of the National Committee for Nuclear Energy, and of the National Council for Science and Technology. In this capacity, unavoidably, he also assumed various high political tasks.

The next seven years were good years for science and particularly for physics. The old institute quadrupled, building many new basic facilities: a tandem, a modern centre for radioisotope production, a nuclear medicine centre, a new laser building, a Mossbauer laboratory, a computing centre. Magurele, the site of the institute, became also a university campus, with a modern building for the faculty of physics, a lyceum, comfortable student hostels and a commercial centre. The economic situation of Romania at that time was healthy enough to allow this development. Moreover, in less than 10 years, the scientific output in physics reached almost two percent of the world output which created an optimistic expectation and attracted young scientists. Ioan Ursu played a decisive and visionary role in this process. In a speech in the fall of 1970, he described in detail the future institute – The Platform of Magurele - that he, together with his predecessor

Hulubei, had contemplated. His national and international status offered a guarantee to the state leaders to allocate funds and the work force necessary to implement these plans. In a way this coincided also with the ambitions and interests of the Ceaucescu presidential couple. The only part of the plan that was not realised until 1977 were of houses and villas that should have lined the road connecting Bucharest to Magurele. This was too much for the spartan future reserved by the party leaders for the population. And no exception was admitted.

Professor Ursu never left his calling for research and writing, authoring over 200 research papers published in prestigious journals and several books written [see References] in collaboration with Romanian and Russian scientists.

His national and international prestige increased steadily. He was elected a member of the Romanian Academy in 1974. An impressive number of national and international societies offered him membership. He was a member of the International Committee of Ampere Association, of the Dubna Scientific Committee, the Soviet Union Academy, and Governor (1972 – 1973) and Member of the AIEA Scientific Committee among other affiliations.

In recognition of his international scientific profile, he was elected as President of the European Physical Society (1976 – 1978). Two large conferences were organised in Bucharest: the EPS-General Conference "Physics and Energy" (1975) and the AMPERE Congress (1982) with the participation of six Nobel laureates. These actions have had a beneficial impact for the visibility and prestige of physics and science in Romania. This can be illustrated by the numerous prizes won by the Romanian teams at various physics Olympiads.

Ioan Ursu was equally concerned with all problems that confronted the economy such as energy and high technology. More than two dozen research institutes were created under his guidance. He was involved directly in elaborating the national nuclear strategy and in the selection of the path to nuclear energy. The choice of the Canadian CANDU power plant proved to be a very wise and profitable one. He was directly involved in various technological aspects of producing heavy water industrially, in the methodology of preparing the reactor fuel and in safety control. A new institute for nuclear technology, a natural uranium fuel processing plant and a heavy water production unit started operation by the end of the 80's. He was interested in establishing a theoretical methodology for isotopic separation based on paramagnetic electron resonance. However this was the time when dark clouds covered Romania which soon reached the brink of collapse. Impoverished by increasing debts and by the low productivity, the economy could no longer sustain itself. A regime of drastic restrictions accentuated the crisis that culminated with the events of December 1989 and the fall of communism.

Ioan Ursu has already lost his position as director of the Institute of Atomic Physics in 1976. The institute has been split into five components under an umbrella called the Central Institute of Physics. Ioan Ursu retained the position of Vice-President of the National Council for Science and Technology as well as other academic and political positions. It was in this capacity that he navigated through the restraints of political, economical, and ideological bounds to help people and institutions to survive and even, in some cases, to prosper. He was very attentive to the needs of anyone who asked for his support. He tried to keep the contacts open outside the country, both East and West, allowing many people to travel abroad. It is amazing how in the midst of the harshest years of the mid 90's, he was able to initiate and support the Balkan Physical Union, becoming its first president in 1986. The Union played an extraordinary role in strengthening the contacts and collaboration between the physicists in the region during the next decade. In spite of the national, religious and political diversity of the area, even in spite of the wars that have shaken a part of it, physics has proved to be an excellent mediator and factor of stability through the rules of logic, fairness and scientific interest.

After the turmoil of 1989, Professor Ursu went through a period of disappointment and uncertainty. An appeal from EPS and a visit of the Secretary General in the spring of 1990 helped his situation a lot though the press was not always very friendly.

Professor Ursu remained close to physics after 1989, helping many people even when his official possibilities were reduced to nil. He remained interested in many areas of physics, including nuclear energy, then laser physics and of course paramagnetic electronic and nuclear resonance. He was very proud to hear that the Cernavoda CANDU power plant was connected to the grid although others are claiming the credit.

Professor Ursu was an extrovert. He liked people and approached them with the openness and naiveté of the Transylvanian country man. He was popular and he liked young people whom he encouraged to take up responsibilities. When I asked him about his greatest achievement, he responded promptly that it was his family, his wife Maria Lucia, and the three children, Horia, Ionut and Ioana, two medical doctors and a physicist.

Many people will not forget him. The Balkan Physical Union, at the General Conference in Istanbul (August 2006), paid homage to his entire activity and role in BPU. One year earlier, in Constanta, he was awarded the title of Doctor Honoris Causa.

It remains for further generations of physicists and historians of science to weigh Professor's Ursu merits from the perspective of his country's development. So far the young scientists, aware or not, make use of what Professor Ursu and many people of his generation strove to implement. This is in fact the natural flow of life.

Professor Ursu passed away quietly and contented that he had fulfilled his duty on earth. ■

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M. Jacob 1933 – 2007

On 2 May 2007, Maurice Jacob, who was President of EPS (1991-1993) died from a heart attack. The EPS community is very sad and expresses its deep sympathy to his family and his friends, at CERN and elsewhere. An homage to Maurice Jacob will be published in the next issue of Europhysics News

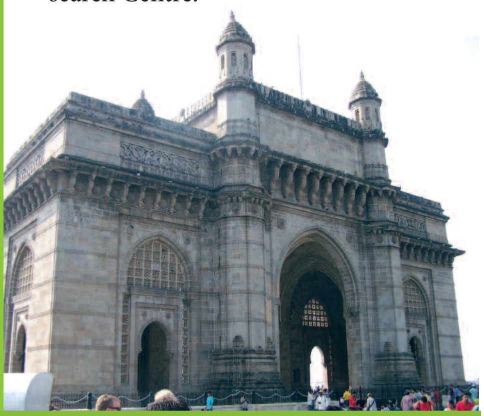
India study tour 2006: experiencing physics abroad [EDUCATION]

Crispijn Jansen, Geert-Jan Besjes and Koen van den Dungen,
Radboud, University Nijmegen, The Netherlands

Every October, 'Marie Curie', the students' association for physics and astronomy in Nijmegen (The Netherlands), organises a two-week study tour. The aim of these tours is to give students an idea of how physics works 'in real life' and, more importantly, in different cultural environments. This year, nineteen students and one associate professor went to India and travelled from Bangalore, via Goa, to Mumbai.

The scientific side of our programme can be divided into two parts: visits to India's major research institutes and visits to smaller universities. The former attract most of the (inter)national funding, enabling them to compete with high-profile European institutes, whilst the latter, lacking the funds for such a level of research, were noteworthy for the opportunity to interact with the local students. The two largest institutes we visited were the Indian Institute of Science (IISc) in Bangalore and the Tata Institute of Fundamental Research (TIFR) in Mumbai. At IISc, we first were given several lectures by staff members of the Department of Astronomy & Astrophysics, giving us new insights into the latest astronomical research. The head of this department, Prof. Arnab Rai Choudhuri, was already familiar to us, being the author of a renowned textbook on plasma physics. After lunch we also visited the laboratories, including the NMR Research Centre.

▲ The EPN group in Mangalore



▲ The gateway in Mumbai

The largest research institute in India is TIFR. Their Department of Astronomy & Astrophysics operates the Giant Meterwave Radio Telescope in Pune as well as a Balloon Facility at Hyderabad to detect cosmic radiation. The Department of Nuclear & Atomic Physics employs both powerful lasers and heavy ion accelerators to simulate extreme nuclear situations in their laboratories.

Speaking with Indian students is one of the best ways to really learn about physics in an entirely different environment. During our visit to the University of Mysore we passed a cosy classroom where students gathered for a lecture. Interested in experiencing their class, we asked our guide whether it would be possible to join the Indian students. The teacher was enthused by our presence and a lively exchange of names, hobbies, experiences and lectures made for some very fruitful interaction. After our supervisor had told the group which courses he gives and how he teaches them, the local teacher followed his example and taught us the Indian approach to Statistical Mechanics.

A different, yet equally valuable, meeting we experienced at the University of Mangalore. The head of the department had prepared an interesting formal gathering with students and staff from their university and our relatively small group. Even more interesting was the informal tea-time that followed the formal gathering, where we discussed religion, marriage, exams and, of course, physics with the Indian students. Unfortunately the faculty had imposed a curfew, because of recent violent actions of some local extremists. We foreigners were hardly in any danger, but the locals were kept safe on the campus. Thus, the evening was spent without their lively and lovely company.

Of course, physics isn't the only good thing in life; we simply had to enjoy the striking Indian landscapes, colourful city centres and beautiful cultural sites. India showed us nature's diversity from lush jungles (with its mosquitoes to keep us company) to impressive plains. One of the cultural highlights was a Hare Krishna temple in Bangalore: enormous, richly decorated and filled with the singing of its many devotees. Other exciting sites include a 40-meter Hindu statue facing the ocean, the beautiful Palace of Mysore and Mumbai's Gateway of India.

In typically Indian fashion, our scheduled flight home was non-existent. Nevertheless, late-night friendly service brought us home with only a few hours delay, although Air France did temporarily lose half our luggage in Paris. Exhausted and satisfied with perhaps too many impressions, our tour, as all good things in life eventually do, came to an end. ■

APFA5: Ties between Physics and Economics [CONFERENCE REPORT]

Anna Carbone, (Torino)

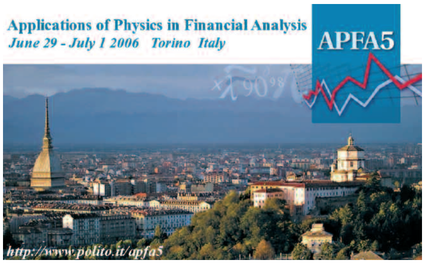
The 5th International Conference on 'Applications of Physics in Financial Analysis' (APFA 5) was held in Torino, from June 29 to July 1 2006. The Conference was chaired by Anna Carbone, Physics Department, Politecnico di Torino, Italy. The program consisted of 30 Plenary Lectures, 42 Oral presentations in 2 parallel sessions and 45 poster presentations. The Conference was attended by more than 180 delegates coming from 30 countries.

The APFA conference series started in 1999 to serve the increasing need to strengthen existing links and build new ties between the physics and economics communities. It is increasingly recognised by both the communities that a number of conceptual and methodological approaches based on statistical mechanics may be employed to understand economic phenomena. In addition to traditional economic notions of coordination via the price system and strategic interaction, models of collective phenomena are now making their appearance in many branches of microeconomics. Other instances of the complexity approaches, familiar to physicists appear in evolutionary game theory, demand theory, behavioural economics and social economics. The analysis of social phenomena, with the introduction of concepts such as scaling and universality, is leading to radically new insights and questions, both theoretical and empirical. All these approaches employ analytical and numerical tools from what is known as the science of complexity, an interdisciplinary approach, initially used for the analysis of systems with strongly interacting subunits in physics and engineering.

The publication of the two issues *"Applications of Physics in Finance"* (*Physica A*, forthcoming) and *"Physics in Society"* (*The European Physical Journal B*, forthcoming) with a collection of 55 papers presented at the Conference is a major result for the advancement and divulgation of the results achieved in the latest years in this interdisciplinary area.

The next edition of the conference will be organized in Lisbon, Portugal, from July 4th to 7th (2007) by the Department of Quantitative Methods, IBS - ISCTE Business School.

Further details and the full-length papers can be found at the website www.polito.it/apfa5. ■

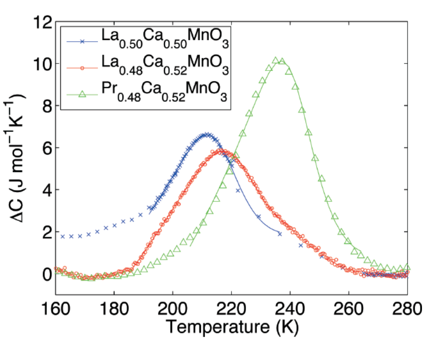


Highlights from european journals

Charge density waves in manganites

Analysis of heat capacity measurements (see Figure) on three manganite compounds, $La_{0.5}Ca_{0.5}MnO_3$, $La_{0.48}Ca_{0.52}MnO_3$ and $Pr_{0.48}Ca_{0.52}MnO_3$ has established that the transition at which the stripe phase appears in manganites is second order, and is accurately modelled as a Peierls transition in a material which is disordered or contains impurities. This is the behaviour expected of a charge density wave in a disordered system, in contrast to the previously accepted picture of charges localised at atomic sites.

Previous studies had concluded that the onset of the stripe phase was associated with the simultaneous onset of ferromagnetism in $La_{0.5}Ca_{0.5}MnO_3$. We have found that the transitions in materials with and without a ferromagnetic signal share a common origin, since the entropy change at the transition is very similar for all three compounds. However, the origin is not associated primarily with magnetic order because, while the magnetisation varies by a factor of 100 between the compounds, the change in entropy remains roughly constant. This overturns the traditional view, and suggests instead that the transition in $La_{0.5}Ca_{0.5}MnO_3$ is driven mainly by a Fermi-surface instability. Our result adds to the growing body of evidence that the stripe and ferromagnetic phases are much more similar than previously thought, and indicates that the colossal magnetoresistance present in manganites is driven by the delicate balance between the ferromagnetic and stripe phase.



These results call for a re-evaluation of the many strongly correlated electron systems which exhibit stripe and checkerboard phases (*e.g.* cuprates, nickelates and cobaltites) in terms of a disordered charge density wave model which produces insulating behaviour without the need to invoke strong electron-phonon coupling. ■

S. Cox, J.C. Lashley, E. Rosten, J. Singleton, A.J. Williams and P.B. Littlewood, "Evidence for the charge-density-wave nature of the stripe phase in manganites", *J. Phys.: Condens. Matter*, **19**, 192201 (2007)

Modelling the inner life of cell adhesion clusters

Adhesion of biological cells to external surfaces is the fundamental process that ensures that multicellular organisms keep their structural identity over time. Moreover cell adhesion is crucial for many physiological processes, including wound healing and the immune response. A cell settles on a surface in a sequence of steps in which the distance between cell and surface gradually decreases from microns to nanometer over the time course of minutes. This process is active in the sense that a cell commits itself to firm adhesion only if it receives suitable signals when establishing adhesion.

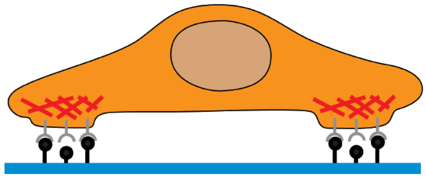
During recent years, it has become clear that these favourable signals also include mechanical cues, which are received through small clusters of appropriate adhesion molecules at the cell-substrate interface. These adhesion molecules appear to be pre-clustered with an average cluster size of three to four molecules, corresponding to a lateral size of nanometres, and then might grow to sizes of 10.000 molecules in a micron-sized cluster, so called "focal adhesions".

The binding dynamics inside focal adhesions is known to be very fast, although it is very difficult to observe it experimentally, due to the 200 nm resolution of optical microscopy. In a recent paper, Thorsten Erdmann and Ulrich Schwarz therefore studied the stochastic dynamics of adhesion clusters of varying sizes in a theoretical model, which is based on well established principles of the physics of cell adhesion.

The two researchers found that for sufficiently small clusters and cell-substrate distances, the adhesion dynamics is characterised by rapid switching between an unbound and a bound state of the adhesion cluster. Such "bistability" has been discussed before mainly in the context of biochemical decision-making, e.g. in cells that decide to divide into two daughter cells.

In contrast, the bistability found in this new study is based on physical binding-unbinding processes and properties of the elastic cellular material. It might allow cells to explore new surfaces by establishing many small and very dynamic adhesion sites. The model also suggests that upon encountering favourable conditions, such transient adhesions could quickly be made permanent by small increases in size and a concomitant reduction in the distance between cell and surface. ■

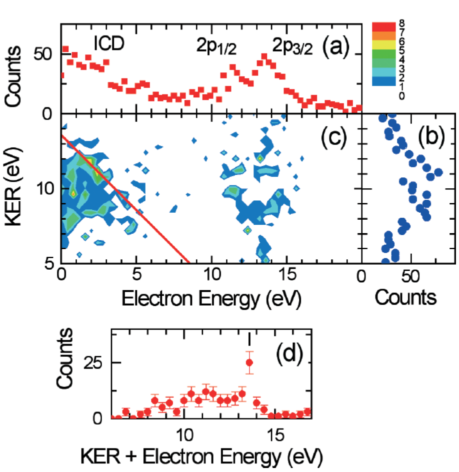
T. Erdmann and **U.S. Schwarz**, "Impact of receptor-ligand distance on adhesion cluster stability", *Eur. Phys. J.* **E 22**, 123 (2007)



▲ This shows a cell (orange, with nucleus) adhering to a substrate (blue, like glass) through two adhesion clusters, each being composed of a number of adhesion bonds, each of which can be either closed or open. It is exactly the stochastic dynamics of opening and closing of these adhesion bonds which is modelled in our work. The structure in red is the actin cytoskeleton which localizes the adhesion bonds into adhesion clusters and also puts them under mechanical stress.

Sequential interatomic decay in argon trimers

We have investigated sequential interatomic decay in the argon trimer Ar_3. Large Van-der-Waals clusters that absorbed X-rays predominantly fragment into singly charged ions and neutrals: highly charged ions are hardly produced. Usually, Auger decay in clusters occurs in the atom that absorbed a photon and thus a highly charged atomic ion is first produced in the cluster. How does this highly charged atomic ion transfer its charge and energy to surrounding atoms in the cluster? In order to clarify the charge and energy transfer mechanism, we have investigated the decay from the argon trimer in the 2p hole state, using electron-ion-ion-ion coincidence technique. The relationship of the electron energy and the kinetic energy release (KER) of the triply-charged argon trimer Ar_3^{3+} in the fragmentation into Ar^+-Ar^+-Ar^+ is shown in the Figure. The distribution of the sum of electron kinetic energy and KER in Figure (d) shows the peak at 13.6 eV. We can assign this peak to the interatomic Coulombic decay (ICD) process following the Auger decay.



The charge and energy transfer mechanism in the argon trimer is found to be as follows. The first-step Auger decay of the 2p hole state in Ar_3 leads to the one-site two-hole state Ar^{++}-Ar-Ar that couples to the two-site satellite state Ar^{+*}-Ar^+-Ar. These states are subject to ICD to the state Ar^+-Ar^+-Ar^+ via the two-site satellite character. This second-step ICD process has been identified unambiguously by the electron-ion-ion-ion coincidence spectroscopy in which the kinetic energy of the slow ICD electron and the KER among the three Ar^+ ions are measured in coincidence. We believe that such sequential interatomic processes that lead to many singly-charged ions can be seen in all clusters, molecules, liquids and solids, especially in biological molecules in living cells. ■

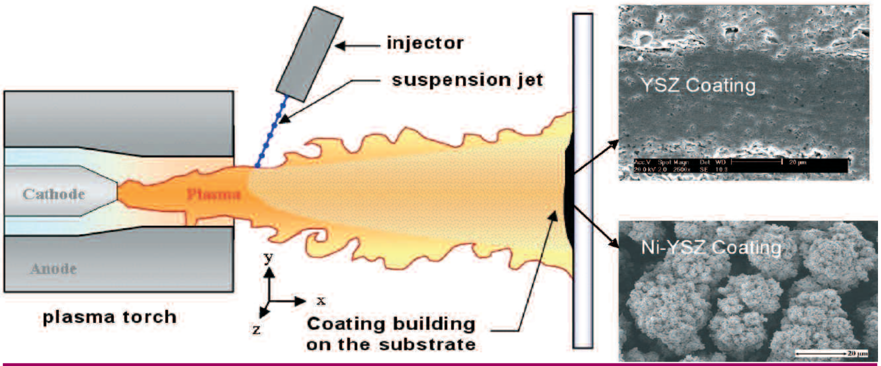
X.-J. Liu, **N. Saito**, **H. Fukuzawa**, **Y. Morishita**, **S. Stoychev**, **A. Kuleff**, **I.H. Suzuki**, **Y. Tamenori**, **R. Richter**, **G. Prümper** and **K. Ueda**, "Evidence of sequential interatomic decay in argon trimers obtained by electron–triple-ion coincidence spectroscopy", *J. Phys. B: At. Mol. Opt. Phys.* **40** F1 (2007)

Plasma spraying for solid oxide fuel cells

The growing energy demand for the settlements of population needs to be balanced by the development of cost-effective and environmentally friendly technologies of energy production. Solid Oxide Fuel Cells (SOFC) have an exceptional potential for use as electric power generation systems since they are fed, at high temperature (~900°C), with oxygen and hydrogen gases to provide electricity and steam cleanly with a high energy efficiency. However, much interdisciplinary research is still carried out that is focused especially on the reduction of the operating temperature of SOFC which leads to a decrease in the cell performance. Research efforts are currently devoted, on the one hand, to the development of new nanoscaled materials (such as apatite or Lamox-type oxides) to improve their electrical properties at low temperature and, on the other hand, to material processing techniques, especially in order to reduce the electrolyte thickness (~10 μm) of SOFC.

Plasma spraying is a promising candidate for such a process because the use of this technology has the advantage of combining the synthesis and consolidation of materials. Thermal plasma-based processes indeed offer high reactive media to treat or synthesize nanomaterials. The combination of the plasma characteristics and those of precursors (liquid, such as suspensions with dispersed submicron particles, and/or solid) which are injected within the plasma, can lead to the desired material properties and microstructure. For example, dense Yttria Stabilized Zirconia (YSZ) electrolytes (15-20 μm thick) have been obtained by using Suspension Plasma Spraying (SPS) (see Figure). A combination of SPS and Solution Precursor Plasma Spraying (SPPS) allows the deposition of finely structured Nickel-YSZ coatings for SOFCs electrode. ■

P. Fauchais, R. Etchart-Salas, C. Delbos, M. Tognonvi, V. Rat, J.F .Coudert, and T. Chartier, "Suspension and solution plasma spraying of finely structured layers: Potential application to SOFCs", *J. Phys. D: Appl. Phys.* **40**, 2394 (2007)



▲ Suspension and Solution Precursor Plasma Spraying (respectively SPS and SPPS) – Yttria Stabilized Zirconia (YSZ) coating obtained by SPS and Nickel-YSZ coating obtained the use of a combination of SPS and SPPS

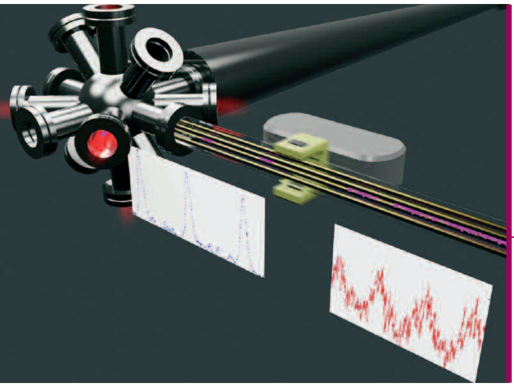
A Mirror to generate a beam

Intense sources of ultracold particles have proven to be a very useful tool for metrology and matter wave optics. In this context, the realization of a slow beam of neutrons through specular reflection on the blades of a rotor [1] has represented a breakthrough leading to many achievements in neutron optics and interferometry experiments. This scheme was also successfully applied to the slowing down of a supersonic beam of Helium, with the aim of realizing a very intense source for neutral atom optics experiments [2].

G. Reinaudi and coworkers have recently demonstrated the implementation of a similar technique with ultra-cold rubidium atoms. In their experimental setup, a laser-cooled atomic packet is sent into a 4.5 m long magnetic guide at a velocity of 1.7 m/s, and is subsequently slowed down by undergoing an elastic collision with a moving magnetic barrier. This magnetic "mirror" is provided by rare-earth permanent magnets mounted on a U-shaped support, and set in motion at an adjustable velocity by means of the mechanical conveyor belt on which it is fixed (see Figure).

This device permits the removal of up to 95 % of the longitudinal kinetic energy of the incident atomic packet. This technique was also extended to a set of packets periodically injected into the guide, resulting in the formation of a continuous, intense and very slow beam of ultracold atoms. Such a beam is a promising tool for atom-optics experiments including matter-wave interferometry, and is also a prerequisite for the achievement of a continuous "atom laser" [3]. ■

G. Reinaudi, Z. Wang, A. Couvert, T. Lahaye, and D. Guéry-Odelin, "A moving magnetic mirror to slow down a bunch of atoms", *Eur. Phys. J.* **D 40**, 405 (2006)



◀ Figure: Laser-cooled atomic packets are injected into a magnetic guide and slowed down by reflection on a moving magnetic barrier. The overlap of the successive slowed packets generates an ultra-slow guided beam.

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Condensed matter theory by computer simulation: from materials to chemical biology

[DOI: 10.1051/EPN:2007009]

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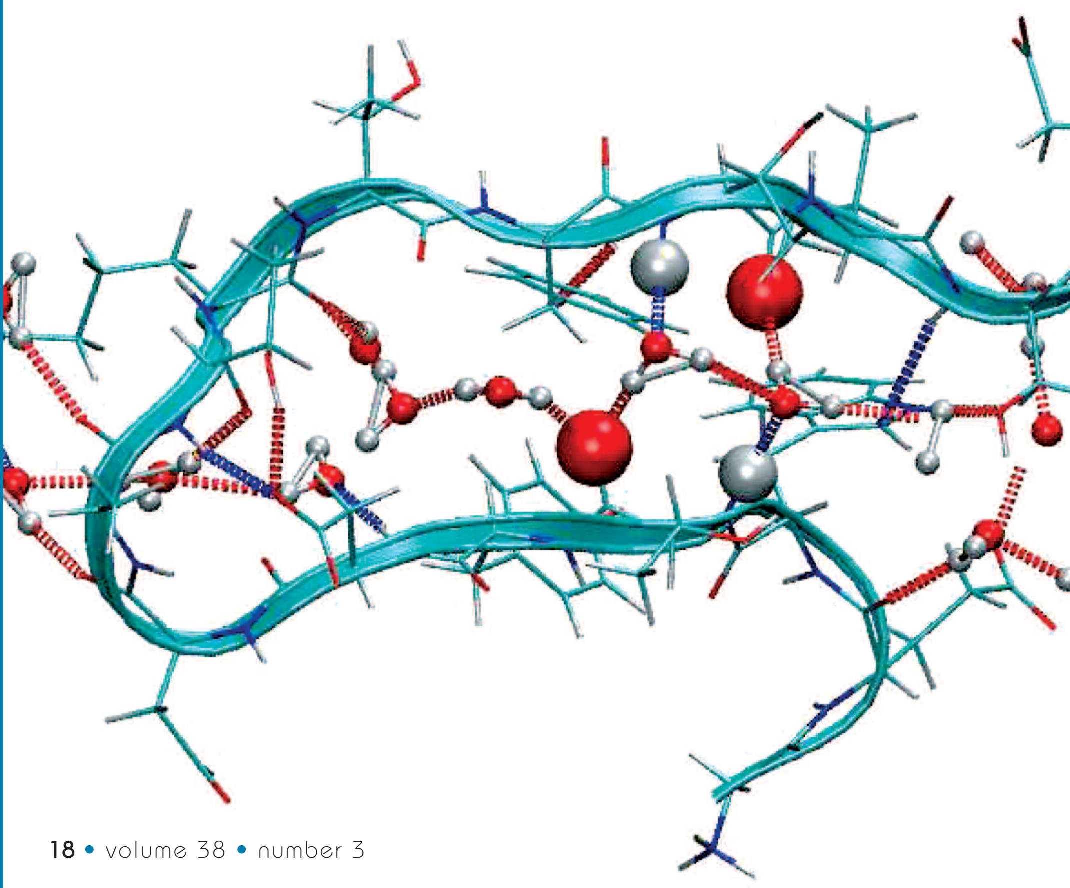
[3] Institut für Physik, Johannes Gutenberg-Universitaet • D-55099 Mainz • Germany

Condensed matter systems, ranging from simple fluids and solids to complex multi-component materials and even biological matter, are governed by well understood laws of physics: on the relevant scales of length and time; the appropriate description would be just the Schrödinger equation for the quantum-many-body problem of the nuclei and electrons interacting with Coulomb forces. Statistical mechanics would then provide the framework to extend this quantum theory of condensed matter towards a statistical description in terms of averages taken at nonzero temperature.

However, this program cannot be carried out straightforwardly: even dealing only with the associated electrons is still a challenge for the methods of quantum chemistry. Similarly, standard statistical mechanics makes precise explicit statements only on the properties of systems for which the many-body problem can be effectively reduced to a problem of independent particles or quasi-particles. Such problems are, for instance, ideal gases, paramagnets, or the multidimensional harmonic oscillator describing phonons in harmonic crystals. While all these problems are useful and educative (we hence teach them all to students to illustrate the spirit of the general theoretical framework) they do not encompass most of the problems of interest in condensed matter physics: the interactions among the considered degrees of freedom introduce nontrivial correlations between them. Systematic perturbation-theory type methods usually do not lead very far, and uncontrolled closed form approximations often fail utterly. A well-known example is the study of the liquid gas transition in fluids: simple theories such as the van der Waals equation and its extensions (*e.g.* the "perturbed chain" statistical associating fluid theory [PC-SAFT] intended to model the equation of state of polymer melts [1]) give rise to spurious loops in the isotherms, fail to describe the critical behavior correctly, and may even predict completely unphysical phase equilibria that do not correspond to any physical behavior of the system but are mere artefacts of the inappropriate approximations [1]. The theory of condensed matter systems contains a never-ending list of such failures!

Hence, until about 50 years ago, condensed matter theory suffered from the basic problem that only a formal framework for the theoretical description in terms of quantum theory and statistical mechanics did exist, while a reliable set of tools that would allow accurate explicit predictions to be made for the static and dynamic properties of these systems from first principles was simply missing!

This unsatisfactory situation has changed fundamentally through the invention of computer simulation, which provides a much more promising approach to these problems. Computer simulation is a novel methodic route allowing the



◄ **Fig. 1:** Typical transition state configuration of the 16 residue terminal fragment of protein G-B1, that forms a so-called β-hairpin structure. The two strands of the backbone, which is represented as a ribbon, are separated by a strip of water molecules. In particular the important backbone hydrogen bonds 3-4 (indicated by large spheres) are bridged by water molecules. Reprinted with permission from [2].

treatment of strong correlations in many-body systems. Starting with the introduction of Monte Carlo (MC) methods more than 50 years ago, and Molecular Dynamics (MD) methods shortly thereafter, the scope of simulation methods has been rapidly expanding, and many exciting technical extensions are still under development, providing broad applications for this new theoretical paradigm of science, and new opportunities for important discoveries. While in the early days of computer simulation suitable computing facilities were very rare and, compared to present-day facilities, very slow and with very small storage capacities, very important discoveries were immediately made, which were very surprising at that time. These surprises include the fact that hard spheres crystallize at a density long before close packing has been achieved, and that dynamic correlations in fluids exhibit long time tails. These discoveries not only have greatly influenced the thinking of theorists and experimentalists alike, but have also been the starting point of a great variety of methodological developments. Now, when a powerful desktop computer is at the hand of every scientist, these advances in simulation methods progress at a breathtaking speed! These methods range from basic many-body quantum mechanics to classical and quantum-mechanical MC and MD methods, both in equilibrium and far from it, and to techniques on a coarse-grained mesoscopic level such as the so-called "Lattice Boltzmann" and "dissipative particle dynamics" methods. The fields to which these methods can be applied are extremely diverse: from fundamental problems in astrophysics and high energy particle physics (such as the transition from the quark gluon plasma to hadronic matter) to basic phenomena of solid state physics (such as magnetism, superconductivity and phase transitions between different crystal structures) and to the rich world of phenomena that complex fluids (liquid crystals, polymers, colloids, micro-emulsions, membranes, etc.) exhibit. Computer simulations in condensed matter now can elucidate properties of materials as well as the major nonequilibrium processes that take place in the living cell.

The school, held at the Ettore Majorana Foundation and Center for Scientific Culture (EMFCSC), Erice (Sicily), in July 2005 emphasized precisely these topics, and was properly entitled *"Computer Simulations in Condensed Matter: From Materials to Chemical Biology"*. The precise selection of topics received special motivation by the research interests of Prof. Mike Klein (Univ. of Pennsylvania), who was honored at this event on the occasion of his 65th birthday. Although in the remainder of this article we cannot describe comprehensively the contents of the lecture notes of this school (which take about 1300 printed pages [2]), we hope nevertheless to summarize concisely where is the front line of current research, using the chapters of these Lecture Notes [2] as a useful guide on this battleground.

Basic tools: classical and quantum simulations methods

As soon as the Metropolis importance sampling method (MC) and molecular dynamics (MD), first proposed in 1953 [3] and in 1957 [4], were introduced, they were applied to elucidate the equation of state of hard disks. Subsequently the study of phase transitions (both of lattice models and of off-lattice systems) has been a very important task of MC and MD methods, since analytical methods are rarely reliable for such problems [5-7]. However, a naive application of sampling techniques to such phenomena will also encounter some problems: at first order transitions, the states corresponding to the two competing phases are normally separated by huge free energy barriers in phase space [5-7]. Since the sampling algorithms do not yield any information on the partition function itself, the information on absolute free energies is lacking and an accurate sampling of the free energy difference between the states is mandatory. This requires (with any standard algorithm) the observation of a large number of transitions back and forth between the two states. Conversely, at second order transitions the growth of the order parameter correlation length (which ultimately diverges when one approaches criticality) and the associated slowness of relaxation ("critical slowing down") have been longstanding obstacles to the quest for highly accurate results [5,6].

It has now clearly emerged [2] that there has been impressive progress with all these problems. A powerful strategy to deal with the problem of critical slowing down is the application of the so-called "cluster algorithms": rather than performing local Monte Carlo updates (of single degrees of freedom) in the systems, one constructs suitable non-local moves. These techniques were first introduced for the Ising model, where, by the Swendsen-Wang and Wolff cluster algorithms (named after the scientists who invented them), one constructs large connected clusters of spins having the same sign with a clever recipe. This recipe is derived such that the resulting clusters are independent of their environment and hence can be overturned at zero energy cost. These concepts have now, to some extent, been carried over to off-lattice systems in the continuum. In this way generic examples such as mixtures of hard spheres with very different sizes, a problem that hitherto was almost intractable, has become accessible to solution [2].

Also the problem of accurately locating first order phase transitions and establishing full phase diagrams of complicated model systems is now well tractable by Monte Carlo methods. Substantial progress has been achieved by "extended sampling" strategies. Many of these advanced techniques that are available today have their roots in the classical "umbrella sampling" [7,8]: the now widely applied "multicanonical Monte Carlo", "extended ensemble averaging", "multihistogram methods", etc. Some variations of these methods, such as "parallel tempering" where a number of systems are run in parallel at a set of neighboring temperatures (or other external control parameters), which are exchanged from time to time, can also be used in conjunction with Molecular Dynamics methods (the latter will be discussed below). While in some of these methods reweighting factors need to be estimated and this is not always straightforward, a particularly convenient approach is the so-called "Wang-Landau sampling" [9]: by a rather simple iteration procedure the energy density of states can be estimated, from which the free energy over the entire temperature range can then be computed. All these methods (and many related ones) are concisely described and put in perspective in Ref. [2]. Applications that are described range from the estimation of interface free energies to the energy barriers that one encounters in the folding of small proteins.

There is a number of technical problems which are more typical of classical molecular dynamics [7] than of MC, although often they are found possibly in a different shape also in MC. The first of these is how to generate averages in ensembles of statistical mechanics other than the microcanonical ensemble: in other words how to couple the system to thermostats, barostats, etc [10,11]. Another typical problem is the simultaneous occurrence of slow and fast degrees of freedom that creates difficulties for an efficient use of MD since straightforward implementations mean a great waste of computer resources. Special techniques, such as the freezing of the fast degrees of freedom by holonomic constraints [12] or multiple time step methods [13], have been developed, starting from the early times. In Ref. [2] a broad range of issues on Molecular Dynamics is spanned, from basic foundations to modern issues that are still under investigation, such as the sampling of conformational equilibria of proteins and free energy barriers.

While the topics discussed so far assume throughout that classical statistical mechanics is appropriate, it is clear that many physical phenomena of interest require a treatment based on quantum mechanics. A special case is the time evolution of a quantum particle in a classical environment. A consistent description can be based on the Wigner formulation of quantum statistical mechanics, allowing the study of transport phenomena in such mixed quantum-classical systems. Complementary approaches on related problems can be based on path integral formulations.

At this point, it should be stressed that the path integral treatment of multi-fermion problems is still hampered by a fundamental problem, the "minus sign problem". Some improvement concerning this problem is probably possible by a resummation over paths, so the stochastic problem of sampling paths is reduced to sampling "graphs". Investigations along such lines already present in ref.[2] could well become a mainstream of research in the future.

Another new type of Quantum Monte Carlo method, the "coupled Ion-Electron Monte Carlo Method", extends the standard variational Monte Carlo approach [14] to obtain a description of electronic structure that provides an interesting alternative to the density functional based Car Parrinello [15] (CPMD) method. The advantage is that the ions can easily be treated fully quantum-mechanically, and this advantage pays off when one studies problems such as the properties of (metallic) hydrogen under high pressure.

Of course, the density functional theory and CPMD are also steadily developing further. Ref. [2] provides thorough reviews of these techniques, from their basic principles to the current state of the art. Particularly interesting extensions concentrate on the possibility to accelerate rare events and compute free energy barriers.

The sampling of rare events, *e.g.* a nucleation process where a huge free energy barrier needs to be crossed to form a critical nucleus of the new stable phase on the background of a metastable phase is a longstanding challenge to simulation. Transition path sampling has been the first scheme introduced to compute the relevant properties without assuming a reaction coordinate. In Ref. [2], both the formal theoretical background ("transition path theory") of this approach and the state of the art of the implementation of this new techniques are discussed, as well as applications to study the pathway of protein folding. (Fig. 1)

Selected applications, from simple fluids to human immune response

This article can only attempt to convey to the reader the flavour of the wide range of problems that one can address today via computer simulation in the science of condensed matter: while in many cases a reductionist approach is needed, progress is achieved, in terms of coarse-grained models, by the imaginative ideas of scientists suitably adapting new models to the problems under study. Coarse-graining means that some small-scale degrees of freedom, which are considered less relevant to the questions considered, are eliminated or else treated in simplified ways. Computer simulation offers the advantage that connections can be established between the models of condensed matter on different scales and the hierarchy from the sub-Angstrom scale, where one deals with effects due to the electrons, up to the mesoscopic and macroscopic scales relevant for living matter.

There are cases where a well-defined separation of scales occurs between relevant and irrelevant degrees of freedom (*e.g.* colloidal suspensions) and others where this is not the case (*e.g.* polymer melts, or biological membranes). In colloidal suspensions, particles of spherical or rod-like or disk-like shape with linear dimensions in the micrometer range, are immersed in a solvent fluid, which acts as a heat bath for the larger colloid particles (but presents also hydrodynamic interactions, and, via ions or polymers dissolved in the fluid, controls also the effective interactions between the colloids). This is a classical case [2] where all the degrees of freedom of the system apart from those of the colloids can be integrated out, and models result which resemble models of simple fluids (the dynamics of the colloidal particles being, however, rather different).

The situation is very different for polymeric systems: a flexible macromolecule exhibits nontrivial structure from the Angstrom scale (chemical bonds) over the coil size (tens of nanometers) to even larger length scales of mesoscale ordering phenomena. Consequently, there does not exist a unique modelling approach to deal with matter formed from such macromolecules. Rather there exists a large diversity of proposed algorithms and different models, as outlined in depth in Ref. [2], to confront fundamental problems of polymer science, such as, for example, understanding which material properties control the "tube diameter" describing the constrained diffusion of polymers in melt (note that polymers "creep" in a snakelike motion along a "tube" that follows their own contour). (Fig 2)

Of course, there are still limitations that have not yet been overcome: while the simulations have contributed much towards the understanding of the slowing down of undercooled simple fluids near the glass transition and while one can also study glassy freezing of very short, non-entangled polymers, the interplay of chain entanglement and glassy relaxation clearly is beyond reach. Similar caveats apply to the studies of spreading and bridging of polymer droplets on substrates - there is still a huge gap between the nanometer length scale and nanosecond time scale of the simulations on the one hand, and the macroscopic scales of the experiment on the other hand. Similar caveats apply to many other problems also discussed in [2], such as defect patterns in liquid crystalline systems, surfactant layers under shear, lipid bilayers with transmembrane proteins modelling biological membranes, etc. However, one should emphasize that for problems of this type, apart from the simulations, there is no reliable theoretical information whatsoever. (Fig 3)

Even in the "classical" problem of spin glasses, a problem heavily debated and well studied for more than thirty years, there is still no relevant analytic theory apart from the mean-field theory of the infinite-range model where every spin interacts with every other spin with random Gaussian couplings.

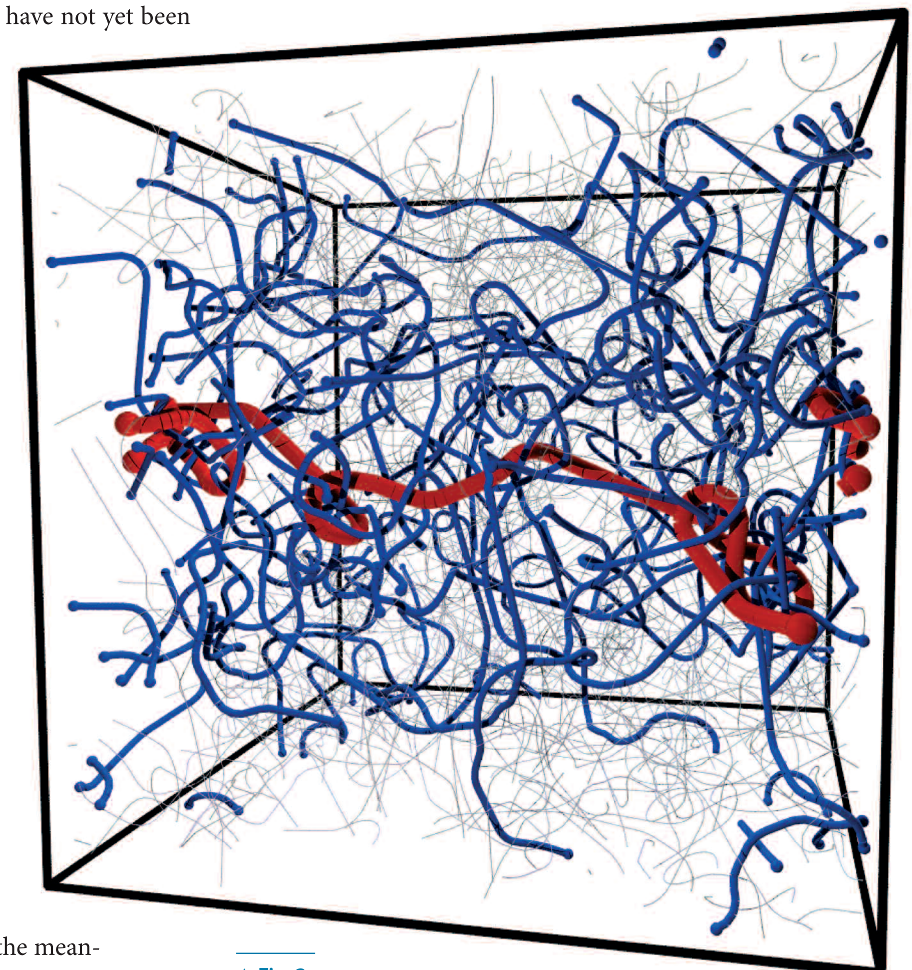
Experiments on these systems can neither probe the order parameter distribution nor the relevant correlations directly, so the guidance from simulations has been absolutely crucial for a better understanding of this problem.

Particularly challenging are the simulation tasks in biologically motivated physics: Drug-target binding necessitates quantum-mechanical approaches for the chemically reactive molecular groups, but the huge size of complex biomolecules in aqueous solution requires a simplified description on long length scales. So hybrid approaches have been introduced that combine ab initio with classical MD in the environment of the reactive groups, by suitable "quantum mechanical/molecular mechanical (QM/MM)" partitioning.

While in this problem one tries to deal with atomistic detail, the problem of evolutionary design of the so-called T-cell receptors that recognize and eliminate tumor cells requires a completely abstract model with no chemical and structural details [2].

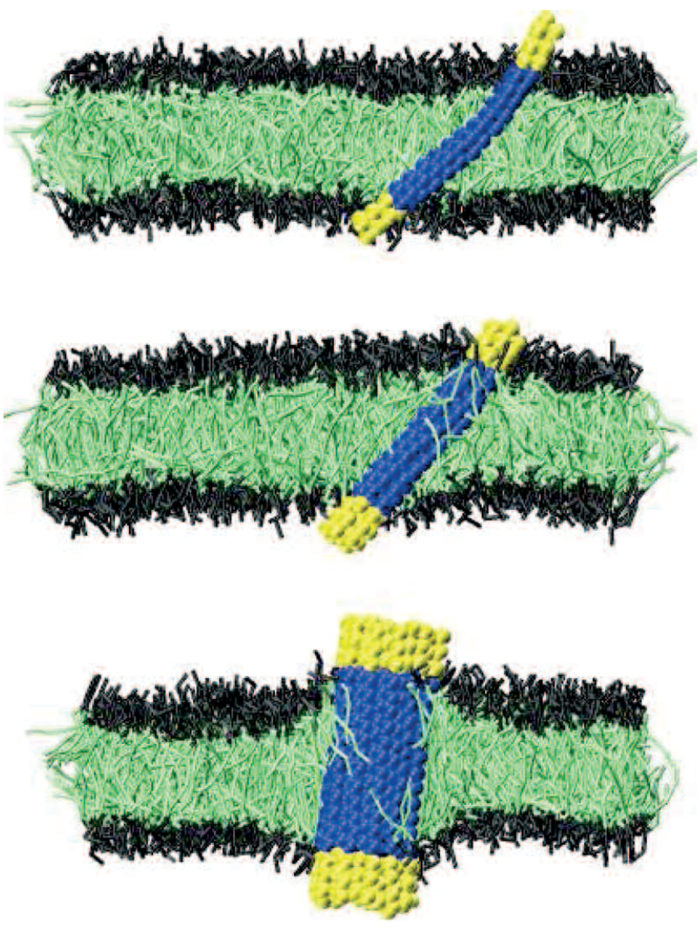
Outlook

We have already emphasized the need to develop mixed (ab initio/classical MD) approaches, where a subsystem is treated ab-initio, and coupled to a classical environment via a transition region where a proper "handshaking" between ···



▲ Fig. 2:
Result of the "primitive path" analysis for all chains in the melt of 100 bisphenole-A polycarbonate chains of N=60 repeat units. The primitive path highlights the geometry of chain entanglement. The red chain is entangled with all those chains whose primitive paths are shown in blue, but not with those shown in light gray. Reprinted with permission from Macromolecules 38, p. 8089(205).

··· both types of simulation is attempted. This is an example of "multiscale simulation", an important paradigm of the field: to combine, in a coherent fashion, complementary methods of computer simulation on vastly different time and length scales for problems of capital interest. *e.g.*, for multi-functional materials hierarchically organized from complex building blocks a molecular simulation may be impossible because of the excessive need for computer time. When one then resorts to coarse-grained models, however, there is a clear need to validate the coarse-grained model by a "mapping" to an atomistic model on smaller scales. In fact, there may also be the need to reintroduce atomistic detail consistently into coarse-grained models ("inverse mapping"). Such techniques have been proposed in the context of polymer melts, but it is clear that the problem is much more general, and far from fully solved. The goal is to develop simulation approaches for complex materials and biological matter that successfully bridge the gap from the small scales of electronic structure calculations to the mesoscopic scales of pattern formation in soft matter (where one uses coarse-grained simulation techniques such as dissipative particle dynamics, multiscale collision dynamics, etc.). While this goal will remain an exciting challenge for many years to come, nevertheless steady and important progress towards reaching this goal can be anticipated. Thus, we can expect that the role of computer simulation as the central and basic method of approach of condensed matter theory will become even much more important in the future. ■



▲ **Fig. 3:** Typical peptide configurations embedded in a coarse-grained model of a biological membrane, for three different peptide sizes. Reprinted with permission from [2].

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Kurt Binder is Professor of Theoretical Physics at the Johannes Gutenberg Universitaat of Mainz. He belongs to the "old horses" generation in the field of Monte Carlo simulations and will receive this year the Boltzmann Medal in the field.

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Toying with physics [DOI: 10.1051/EPN:2007010]

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In the early 19th century the popularisation of science became a vogue, expressed in books that often took the form of "conversations on natural philosophy". They may have echoed the discourse of the classical dialogue of debate but this was more the conversation of the drawing-room, albeit in the stilted parlance of the time.

The top, my boy is a subject which the great Mantuan bard did not consider beneath the patronage of his muse. (anon., quoted in [1])

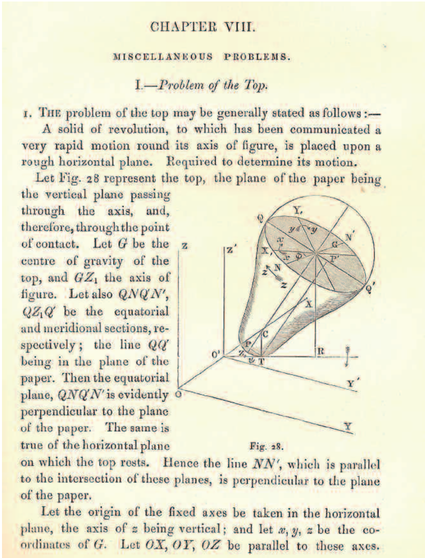
Such lessons were aimed at future scientists ("boys"), the workers ("operatives") and even the gentler sex ("little housewives"). Of three particularly influential texts [1,2,3], two were by women [2,3], one of whom preferred to remain anonymous for some time. The third, written by the early cancer researcher John Ayrton Paris, was splendidly entitled "Philosophy in Sport made Science in Action, being an Attempt to implant in the Young Mind the first Principles of Natural Philosophy by the aid of Popular Toys and Sports of Youth". Examples of the many playthings included as "instruments of philosophical instruction" are the seesaw, the kite, the top, and the Jew's Harp.

"*And is it then possible", said the vicar, in a tone of supplication, "that you can seriously entertain such a wild and, I might add, kill-joy scheme?"* [1]

Paris' kill-joy scheme ran to many editions and imitations and helped found a pleasant tradition that was followed in later years by such popularisers as C. V. Boys in his lectures on soap bubbles, an early version carrying the flowery title "Soap-bubbles, their Colours and the Forces which mould them: Being the Substance of many Lectures delivered to Juvenile and Popular Audiences with the Addition of several new and Original Sections" [4]. Perhaps it faltered in the period of high seriousness about physics in the mid-20th century; nuclear physics had no place in the nursery. But today it emerges afresh in the minds of our physics teachers at every level (for a recent collection of experiments on soap bubbles see the books by Rämme [5]). Museum shops offer a variety of such diversions, from cheap plastic to executive-toy chrome, but many can be found in the kitchen, the toolbox and the sewing cabinet, or are easily constructed. Toys have become part of our cultural heritage, as one observes in archaeological digs, in the items for sale in antique shops, in museums, and the inclusion of the "slinky" in the US Postal Services "Celebrate the Century" series of postage stamps.

◄ **Fig. 1:** Slinky on a US postage stamp commemorating the ``Slinky craze" of 1945.

One of the present authors essayed a lecture [6] on such teasing trivialities at the "International Conference on Theoretical and Applied Mechanics" in Warsaw (2004). An eager audience overflowed the capacity of the lecture theatre. At the preceding congress in Chicago (2000), as part of a Science Teachers Day, Professor Raymond C. Turner of Clemson University told an appreciative crowd of local physics and science teachers about using toys to teach. Many in the audience were very conversant with this mode of instruction, but keen to learn more.



CHAPTER VIII.

MISCELLANEOUS PROBLEMS.

I.—*Problem of the Top.*

1. The problem of the top may be generally stated as follows:—
A solid of revolution, to which has been communicated a very rapid motion round its axis of figure, is placed upon a rough horizontal plane. Required to determine its motion.

Let Fig. 28 represent the top, the plane of the paper being the vertical plane passing through the axis, and, therefore, through the point of contact. Let G be the centre of gravity of the top, and GZ_1 the axis of figure. Let also $QNQ'N'$, QZ_1Q' be the equatorial and meridional sections, respectively; the line QQ' being in the plane of the paper. Then the equatorial plane, $QNQ'N'$ is evidently perpendicular to the plane of the paper. The same is true of the horizontal plane on which the top rests. Hence the line NN', which is parallel to the intersection of these planes, is perpendicular to the plane of the paper.

Fig. 28.

Let the origin of the fixed axes be taken in the horizontal plane, the axis of z being vertical; and let x, y, z be the coordinates of G. Let OX, OY, OZ be parallel to these axes.

▲ **Fig. 2:** A page from Jellett's *Treatise on the Theory of Friction* (Macmillan, London, 1872) where *Jellett's constant* is introduced.

Childlike absorption

Many famous personalities of physics have had a taste for toys and tricks. Von Kármán [7] described Prandtl's "childlike absorption":

In subsequent months I came to know Prandtl quite well. He was a man of strange contrasts. Sophisticated and gifted in science, and a great teacher on a person-to-person basis, he was nonetheless naïve about life and childlike in behavior. He could not pass a toy in a shop, for instance, without curiously fingering it, and he was spell-bound by routine magicians tricks. Once at a party the guests decided out of fun to test Prandtl's well-known love of toys. In one corner of the room somebody placed a child's gyro, in such a position that it would be in full view. Everybody awaited Prandtl's arrival to see whether the professor would live up to expectations and go directly to the toy. He didn't disappoint them. As soon as he entered the room and his eye fell on the toy, he had no interest in anything else or in anyone at the party. It was almost half an hour before Prandtl realized that the party had formed around him and that everyone was secretly enjoying his childlike absorption.

Other well-known scientists who have written about the analysis of toys and games include G.-G. Coriolis, today principally known for the acceleration that bears his name, but a distinguished mechanician who in 1835 wrote "Théorie mathématique des effets du jeu de billard"; F. Klein and A. Sommerfeld, •••

▲ **Fig. 3:** The so-called Russian *rattleback* in which the two small control masses (shaped as turtles) can be adjusted to create an asymmetry that dramatically affects it motion.

••• seminal figures of the late 19th and early 20th century in mathematics and physics, respectively, who collaborated on "Über die Theorie des Kreisels", publishing all four volumes in Leipzig between 1897 and 1910; H. Bondi, J. L. Synge, and K. Stewartson all wrote about spinning tops and so on. This tradition of studying toys seriously has, fortunately, survived to the present day, and we find in the current literature and in premier journals contributions on the "Levitron" [8], on "Newton's cradle" [9] (and references therein), and on "Euler's disk" [10].

Maddening mechanics

With so much to choose from, we shall concentrate on mechanics, a subject misleadingly presented as rather trivial in elementary physics classes.

The tractability of many problems of rational mechanics may be its attraction: even the spinning rigid body bows to theory for the special cases usually considered. But add a bit of asymmetry, or a dash of friction or other contact forces, and you soon have a recipe for strange, counter-intuitive gravity-defying behavior. Unpalatable mathematical formalism is needed to explain it.

Many effects were well known already in the nineteenth century. For example, a *spinning* top will rise to the vertical "sleeping" position: why? In his popular work "Spinning Tops" John Perry (1890) waxed sarcastic on the subject of Cambridge men who thought they surely understood but had forgotten the details. It had something to do with the action of friction on the rounded tip of the top - it is fairly evident that reducing it to a point removes the hope of an explanation. For a proper elucidation Perry was directed by another Irish phyicist, George Francis Fitzgerald, to the work of his father-in-law. John Jellett's "Treatise on the Theory of Friction" contains much wisdom on the role of friction that endures today, in particular "Jellett's constant".

The constant arrives unheralded in a section of miscellaneous applications (see Fig. 2). It is the result of judicious approximation: if the rotation about the symmetry axis of the top is regarded as dominant, an additional conserved quantity emerges. Jellett used it in a neat argument to show that, as friction reduces the energy of the top, it must rapidly bring it to the upright position.

But with both friction and asymmetry we are still in real trouble. The classic example is the celt (pronounced "selt"), rattleback or wobblestone, guaranteed to stun a class that sees it reverse its direction of rotation on an overhead projector. In his inspiring book "The Flying Circus of Physics" Jearl Walker writes [11]:

> *Some of the stone instruments made by primitive men... display curious personalities...These stones, called celts, are generally ellipsoidal in shape. When you spin them about a vertical axis some behave as you would guess, but others act normally only when spun in one direction about the vertical. If you spin them in the other sense, the rebellious stones will slow to a stop, rock for a few seconds, and then spin in their preferred direction...If you tap one of these stones on an end, ... it will rock for a while. But soon the rocking ceases, and the stone begins to rotate about the vertical axis. What causes such personalities?*

Figure 3 depicts a neat variation. A "tunable" rattleback, commercially known as the Russian rattleback (probably because of the style of decoration). The two small turtles may be rotated on the "deck" of the otherwise completely symmetric "hull". When they face one another, the object rotates with equal ease in the clockwise or the counterclockwise direction. However, turn the turtles so that they are perpendicular to the axis of the hull, facing in opposite directions, and the mysterious behavior emerges at once. They like to ride in the forward direction, and wobble and reverse direction if spun so they are riding backwards.

Perry describes another variation: an ellipsoidal stone spun on a surface, about one of its shorter axes: it staggers into the upright position, spinning about its long axis. A further elaboration is the additional end-to-end asymmetry of an egg, which, if spun with its blunt end down will flip over, and spin on its sharp end. This is the same behavior seen in the "Tippe-Top" toy, which has fascinated amateur and professional physicist alike. A famous snapshot (Fig. 4) shows Wolfgang Pauli and Niels Bohr experimenting with the apparent angular-momentum-reversing behavior of the tippe-top.

According to Perry, Lord Kelvin would experiment with oddly shaped stones when he went to the seaside, exploring such peculiar dynamics. He was also fond of eggs, for undergraduate demonstrations, baffling the class with the different properties of identical eggs (one of which was hard-boiled).

In a modern study of eggs worthy in its erudition of an emeritus Cambridge professor, Keith Moffatt has addressed not only some of these extraordinary feats, but also the astonishing capacity of an egg to jump vertically in the course of its rotational manoeuvres [12].

Moffatt came to the problem via a simpler one, that of the Euler disk. This is just a metal disk, the heavier the better. When spun on a flat surface it gradually slows, but its audible frequency of rotation increases dramatically. It rises inexorably towards a crescendo and stops abruptly, like the best symphonies.

Who said dissipation causes motion to die away slowly? Here it provokes a mathematical crisis called a finite-time singularity, important in modern fluid dynamics.

In relatively modern times, the rotational toy that has made the biggest move in the stock market is surely the "yo-yo". Like many of our toys it has a pedigree measured in millennia, and there have been periodic crazes in the modern era. (Invest now.) Another device of ancient origin is the diabolo. James Clerk Maxwell was given one as a child and took it with him to Cambridge (Fig. 5).

All of the above is certainly abstruse - some would say that it is more of a lesson in humility for the teacher than elementary physics for the pupil. So let us retreat to something simpler - "Newton's cradle", as shown in Figure 6. A ten-second experiment with a ten-second explanation in terms of conservation of energy and angular momentum? But there is a greater lesson to be learned: do the experiment, and make careful observations...

We observe that, if one ball is pulled aside and released, it is not precisely true that only one ball is ejected from the other side. Merely some misalignment in manufacture? It turns out that the cause is not to be found there, but rather in the finite compressibility of the balls, which renders collisions non-instantaneous. A compressive elastic pulse of finite width is propagated down the line. When it ejects the last ball, the previous two are still slightly compressed together, so they fly apart too in a clearly visible displacement (the remaining displacements are not usually discernible). Recognizing this, we see that the subsequent motion cannot long conform to what is expected (and taught by many). Indeed it does not, and several papers address this motion; see [9] and references therein. To observe it unmodified by air drag, build a big Cradle, and rock it. Discarded bowling balls would be good.

Funny fluids

Fluid mechanics has its share of toys, executive and otherwise. The "Ooze Tube" and its variants allow one to watch the coiling of a thread of viscous liquid falling through a small circular hole, see Figure 7. Barnes and Woodcock [13] call this the "liquid rope-coil effect". In his paper at the "12th International Congress of Applied Mechanics", held at Stanford University in 1968, the father of modern fluid dynamics, G. I. Taylor showed and analyzed examples of instabilities of jets, threads and sheets of viscous fluids.

The thin thread with a circular cross-section coils neatly into a growing mound. A flat ribbon, on the other hand, will fall in layers. When placed horizontally, and thus constrained to move two-dimensionally, the thread will buckle. Taylor gives the following explanation [14]:

> *The reason for the instability is clear. If the stream is very thin, the longitudinal compression acts in the same way as end compression in a thin elastic rod. The rod becomes unstable at a certain load, and less force is needed to move the ends towards one another when the rod is bent than when it is straight. This is called Euler instability.*

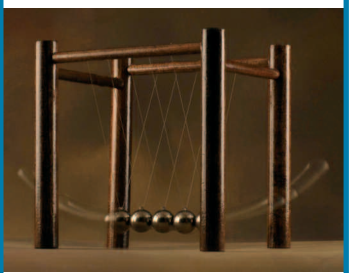
Experiments [13] show that the effective height of fall and the frequency of coiling of a viscous thread are proportional. Is this clear from elementary considerations? Simple dimensional analysis, using just the coiling frequency, the height of fall, and the acceleration of gravity, inevitably yield a frequency inversely proportional to the square root of the height - not at all the observed relationship. However, introduce the kinematic viscosity of the liquid, as would immediately be suggested by simple fluid mechanics, and dimensional analysis yields two dimensional groups, one of which is a "Reynolds number" for the flow. For small values of this dimensionless number or slow flow, we obtain a coiling frequency proportional to the fall height as observed.

The so-called "Brazil nut effect" is the observation that in a mixture of granular material of different sizes, *e.g.*, a can of mixed nuts, the large particles are often observed to end up on top. One intuitive explanation is that when the container is shaken, the small particles flow to fill in voids with greater probability and facility than large particles, hence achieving ···

▶ **Fig. 4:** Two giants of modern physics, Wolfgang Pauli and Niels Bohr, fascinated by the counter-intuitive behavior of the tippe-top. (Photograph by Erik Gustafson, courtesy AIP Emilio Segre Visual Archives, Margrethe Bohr Collection) (reproduced with kind permission of AIP).

▲ **Fig. 5:** Maxwell's diabolo. (Photograph courtesy of the University of St. Andrews.)

▼ **Fig. 6:** Newton's cradle.



··· segregation. There is a mechanical toy, the "Sand wand", that exploits this effect, see Figure 7. Enclosed in a transparent cylindrical tube is a roughly monodisperse granular material and a single steel ball that almost spans the tube. Move the ball, one is instructed, to one end of the tube. Gentle manipulation, rotation, tapping, and so on will not do the trick. A few sturdy shakes with the rod essentially vertical and the desired result is achieved, the glittering ball emerging from the smaller grains and settling on top of them.

A perennial favorite is the "Cartesian diver" or sometimes Cartesian devil - although the attribution to Descartes is, apparently, misplaced - often artfully crafted as a small demon-like creature, submerged in a vertical glass cylinder filled with water, see Figure 7. The cylinder has a flexible membrane at the top. Depress the membrane and the diver descends as if magically heeding instructions from a distance. Release the pressure and he ascends. With a bit of practice he can be made to swirl and dance in the water column. What is the source of this magic? The diver is constructed with a small air-filled chamber inside, open at the bottom and there in contact with the water. When the water column is compressed, the air pocket within the diver is much more easily compressed. The buoyancy of the diver (and the air pocket with him) is reduced and he descends. As with the rest of us, already struggling to stay afloat, a bit more pressure applied from above and we are totally submerged!

Positive play

There is a creative playfulness to good science, and using toys in instruction seems to bring this full circle. They are approachable, intuitive, familiar, we are tempted to say "easy". We feel that we understand how they work. We certainly know how we expect them to work. When they turn out to challenge our intuition and our deepest analytical abilities, do we become insecure or intrigued? Hopefully the latter and, hopefully, that curiosity breeds interest, engagement, creativity, and, ultimately an affection for scientific inquiry. ■

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Denis Weaire is Erasmus Smith Professor of Natural and Experimental Philosophy at Trinity College Dublin and has a keen interest in the history of Physics. Together with **Stefan Hutzler**, who is a lecturer at TCD, he has written a book on the Physics of Foams, containing further examples how child-like fascination (in this case with soap bubbles) can be turned into science.

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► **Fig. 7:** Fluid mechanical toys. **up**, the "Ooze Tube" illustrating the instability of a viscous liquid thread. **Center**, the "Sand wand" - how does one move the steel ball to the to top of the granular material in the tube? **down**, the "Cartesian diver" illustrating simple principles of buoyancy.

Bounded modes to the rescue of optical transmission

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In the beginning of the 19th century, T. Young and J. Fraunhofer built the first optical diffraction gratings and showed the role of optical diffraction in their behaviour. Since that time, diffraction gratings have been used in a broad range of technological applications, from the earlier accurate optical spectrometers to the recent integrated optical devices. They are also used in a broad range of wavelength from X-ray to microwaves. In this context, diffraction gratings have been the cornerstones of many publications for almost two centuries. Surprisingly, nowadays the subject is far from being exhausted.

Every student knows that a grating can spread a white light beam from an incandescent lamp into a continuous spectrum of colors. For a grating made with a one-dimensional lattice of thick-thin wires, this "rainbow" is duplicated many times, each one corresponding to a diffraction order m (See Fig.1 for instance). These basic behaviours of diffraction gratings can be easily understood by the conservation of light momentum such as

$$\vec{k}_s = \vec{k}_i + \vec{K} \tag{1}$$

where $\vec{k}_s$ is the momentum of the scattered light, $\vec{k}_i$ is the momentum of the incident light, and $\vec{K}$ is a vector of the reciprocal lattice of the grating such that $\vec{K}\cdot\vec{a} = 2\pi m (m \in \wedge)$, where $\vec{a}$ is the basis vector of the lattice. The general behaviour of optical grating results from this basic assumption. For instance, in Fig.1, one considers a reflecting grating. An incident light i is then scattered into three diffraction orders. The zero order ($m = 0$) is known as the specular beam. In Fig.1, two other orders are considered, $m = 1$ and $m = -1$.

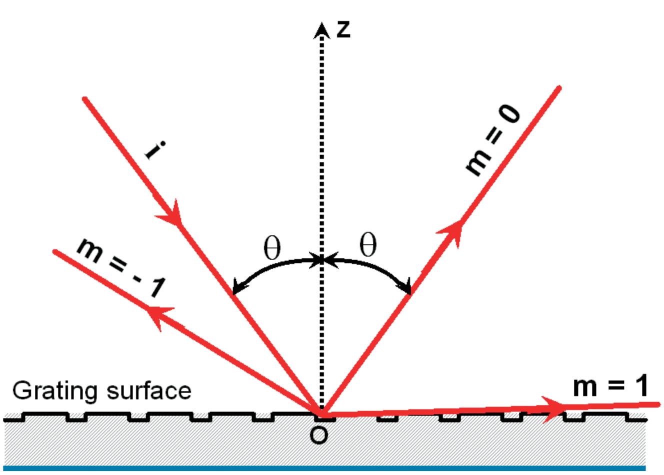
Wood anomalies

In 1902, R. W. Wood observed some unexpected patterns in the spectrum of light resolved by optical diffraction gratings [1]. The Wood spectrum presented many unusual rapid variations of its intensity in certain narrow wavelengths bands. As a consequence, these effects unexplained by ordinary grating theory were named "Wood anomalies".

In 1907, Lord Rayleigh proposed an explanation of those anomalies [2]. Considering for instance the case of the Fig.1, one notes that the order $m = 1$ becomes tangent to the surface grating before disappearing. In such a case, the light momentum component along the Oz axis of a diffracted order m, *i.e.* $k_{z,m}$, becomes imaginary right after having been cancelled. Then, the diffracted order becomes evanescent (non-homogeneous order). When $k_{z,m}$ is real, the diffracted order is free to propagate along the Oz axis (homogeneous order). In the present case, as the order $m = 1$ turns to be non-homogeneous, its energy will be redistributed over the other orders. As a consequence, the diffracted beam intensity of the specular beam ($m = 0$), for instance, increases just as the diffracted order $m = 1$ vanishes. For an incidence θ (see Fig.1), a diffracted order m becomes non-homogeneous for wavelengths greater than a specific value, the Rayleigh wavelength, for which an anomaly occurs. One then talks about a Rayleigh anomaly.

Around 1938, U. Fano proposed another explanation [3], where the anomalies are related to a resonance effect. Such a resonance comes from a coupling between an eigenmode of the grating and a non-homogeneous diffraction order (one also talks about a resonant diffraction order), *i.e.* after it vanishes for wavelengths greater than the corresponding Rayleigh wavelength.

From an experimental point of view, gratings can then show some very complex behaviour often hard to explain in details without the use of Maxwell's equations. In addition, solving Maxwell's equations in order to study the electromagnetic diffraction quickly becomes a difficult problem, even with simple geometries. Except for some simple and powerful analytical works, such as those from Lord Rayleigh or U. Fano, it will be necessary to wait until the Sixties and the beginning of computer calculation to observe significant progress in the Wood anomalies comprehension. For instance, one can underline the first fundamental numerical results of Hessel and Oliner in 1965 [4], and Maystre and Nevière in 1977 [5,6]. Hessel and Oliner presented a wide study of the eigenmode resonance role in Wood anomalies [4]. They have shown that depending on the type of periodic structure, the two kinds of anomalies *i.e.*, Rayleigh anomalies or resonant anomalies may occur separately or are almost superimposed.



▲ **Fig. 1:** A reflecting optical grating. i is the incident light beam. The light beams labelled m are some of the diffracted orders and θ is the angle of incidence.

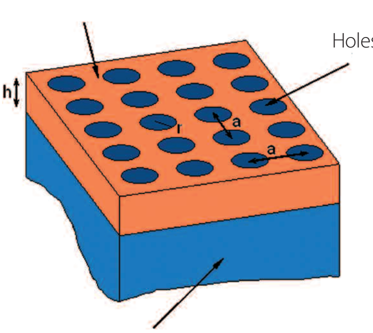
Maystre and Nevière studied specific cases of such resonant anomalies [5,6]. For instance, they presented a wide study about "plasmon anomalies", which occurs when the surface plasmons of a metallic grating are excited [5]. They also considered an anomaly that appears when a dielectric coating is deposited on a metallic grating, and corresponds to guided modes resonances in the dielectric layer [6].

It is important to underline that, in some recent publications, some authors improperly reduce the Wood anomalies to the Rayleigh anomalies only. It is important to recall that the Wood anomaly concept covers the resonant anomalies (Fano anomalies) and the Rayleigh anomalies at the same time. In addition, the resonant part of the phenomenon can imply many kinds of resonances and not only the surface plasmons resonances. Amazingly, thirty years after the pioneer works, in the early 21st century, the experimental and theoretical interest in these subjects has not dried up.

Optical transmission in a nanostructured slab

In 1998, Ebbesen *et al* [7] reported on optical transmission experiments performed on periodic arrays of subwavelength cylindrical holes drilled in a thin metallic layer deposited on glass (see Fig.2). These experiments renewed the motivation for investigating metallic gratings, in particular those with a two-dimensional lattice. The most attractive characteristic of their results was the peculiar wavelength dependence of the transmission (see Fig.3). The latter was defined as the ratio between the energy of the specular transmitted beam ($m = 0$) only and the energy of the incident beam. After these first experimental observations, the role of the thin metallic film surface plasmons (SPs) was put forward in order to explain the peculiar wavelength dependence of the transmission [7].

A surface plasmon on a plane surface is a non-radiative electromagnetic mode, associated with a collective excitation of electrons at the interface between a conductor and an insulator. In this way, a surface plasmon cannot be excited directly by light, and it cannot decay spontaneously into photons. The non-radiative nature of SPs is due to the fact that interaction between light and SPs cannot simultaneously satisfy energy and momentum conservation laws. Moreover, the momentum conservation requirement can be achieved by roughening or corrugating the metal surface, for instance. It is exactly the situation in those devices. In this case, the transmission peaks were interpreted as SPs resonances [7]. Surprisingly, this approach seems to have been suggested independently of the knowledge of some earlier works about the reflecting one-dimensional gratings. Then, the first attempt to understand the Ebbesen experiments has missed some important earlier results of the optical gratings study.



◄ **Fig. 2:** The typical bidimensional array of subwavelength holes.

In this way, in these first interpretations, the exact role of SPs was not clearly assessed, and many questions remained to clarify completely the scattering processes involved in these experiments.

As a consequence, some other explanations had been developed which could compete with the SPs model. For instance, it was suggested that these phenomena could also be described in terms of cavity resonances taking place into the holes [8]. More recently, T. Thio and H. Lezec had also suggested a diffracted evanescent wave model [9].

In addition, some doubts against the SPs hypothesis relied on some experimental results about subwavelength hole arrays made in non-metallic films. Though SPs cannot exist, the transmission pattern was found to be very similar to that obtained with a metallic film [9]. Surprisingly, the very fact that the typical transmission pattern can be observed even in non-metallic systems convinced some authors to fully reject the SPs hypothesis and rather consider models involving nonresonant evanescent waves diffraction. To our knowledge, this point of view is not supported by recent results. In fact, the SPs must be replaced by other kinds of eigenmodes in the nonmetallic cases.

As a consequence, despite alternative theoretical interpretations, a large experimental consensus, many theoretical results, tend to prove that the SPs interpretation was correct in the metallic films cases, and must be extended to a bounded mode interpretation in the most general cases [10-12]. It is only the transposition of the 1960's results about one-dimensional reflection gratings to bidimensional transmission gratings.

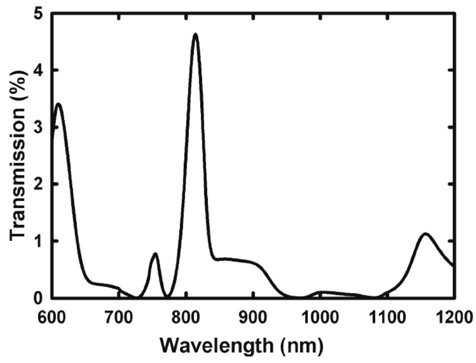
Let us clarify this.

Bounded modes and transmission

Basically, the gratings considered here are simply drilled slabs. In this case, a bounded mode, *i.e.* an eigenmode of the grating, is an electromagnetic field configuration such that the field is trapped along the slab. The mode can propagate along the slab, but not elsewhere. The amplitude of the field decays then, exponentially from each side of the slab. Typically, two amplitude patterns exist, which correspond to symmetric and antisymmetric modes. As the thickness of the slab increases, in some cases, the modes can refer to pure surface modes (Fig.4), *i.e.* both slab interfaces are decoupled. Surface plasmons are such modes for instance.

As previously suggested, bounded modes cannot be excited directly by incident light or decay spontaneously into photons. Moreover, the coupling between the outside electromagnetic field and the bounded modes is allowed by the use of rough or corrugated surface, as in the present case. The eigenmodes, and their coupling with outside light, can be described mathematically as follow.

As in quantum mechanics, a scattering problem can be treated in electromagnetism *via* the use of the scattering matrix formalism (S matrix). In such a representation, it is assumed that the electromagnetic field can be described by two super-



▶ **Fig. 3:** Computed optical transmission of a thin gold film (200 nm) deposited on glass. 100 nm is set for the radius of each hole and the lattice parameter is taken to be a = 700 nm.

vectors $|F_{in}\rangle$ and $|F_{scatt}\rangle$ (with the use of "ket" representation), which correspond to the incident electromagnetic field that lit the studied device and to the field scattered by the device. For instance, each component of these vectors corresponds to a specific diffraction order. Then, incident and scattered field are linked via the scattering matrix defined as

$$|F_{scatt}\rangle = S(\lambda)|F_{in}\rangle \tag{2}$$

so that $S(\lambda)$ contains all the physical information about the studied device, such as a diffraction grating. In addition, it can be shown that $S(\lambda)$ can be explicitly defined from the Maxwell's equations. For instance, the simulations in our papers are based on such a method, which combines scattering matrix formalism with a plane wave representation of the fields. This technique provides a computation scheme for the amplitude and polarization (s or p) of reflected and transmitted fields in any diffracted order.

A fundamental key to the understanding of diffraction grating phenomenology is to define the eigenmodes of the studied device. Eigenmodes then obey the homogeneous equation

$$S^{-1}(\lambda_p)|F_{eigen}\rangle = 0 \tag{3}$$

in such a way that the eigenmodes can also be defined by the poles λ_p of the scattering matrix. Then, the poles are the solutions of the equation

$$\det\{S^{-1}(\lambda_p)\} = 0 \tag{4}$$

If we extract the singular part of $S(\lambda)$ corresponding to the eigenmodes of the structure, we can write $S(\lambda)$ in an analytical form as

$$S(\lambda) = \sum_p \frac{R_p}{\lambda - \lambda_p} + S_h(\lambda) \tag{5}$$

This is a generalized Laurent series, where R_p are the residues associated with each pole λ_p. One notes that $\lambda_p = \lambda_p^R + i\lambda_p^I$ are complex numbers, and that the imaginary part λ_p^I can be linked to lifetimes of the eigenmodes. The divergent behaviour of the fractional terms underlines the resonant character of the eigenmodes (one talks then about the resonant terms of the S matrix). $S_h(\lambda)$ is the holomorphic part of $S(\lambda)$ which corresponds to purely non-resonant processes. Ideally, in the vicinity of a specific pole, the holomorphic part can be assumed to be almost constant. Then, as the amplitude $s(\lambda)$ of a specific diffraction order is related to an element of the scattering matrix, the intensity $I \propto |s(\lambda)|^2$ of an order can be easily derived. One then obtains

$$I_F = \tilde{I}_0 \frac{(\lambda - \lambda_z^R)^2 + \lambda_z^{I\,2}}{(\lambda - \lambda_p^R)^2 + \lambda_p^{I\,2}} \tag{6}$$

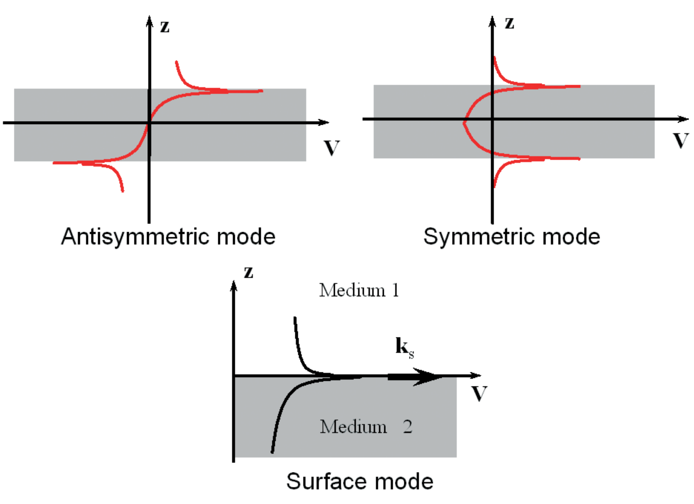
where $\lambda_z = \lambda_z^R + i\lambda_z^I$ is the complex zero of $s(\lambda)$ in the vicinity of λ_p in the complex plan. This function leads to a typical asymmetrical profile, a Fano profile, related to a Fano resonance. A typical Fano profile appears in Fig.5 (black curve). Now, if the holomorphic part is considered as negligible, one gets the following expression of the amplitude

$$I_{BR} = I_0 \frac{1}{(\lambda - \lambda_p^R)^2 + \lambda_p^{I\,2}} \tag{7}$$

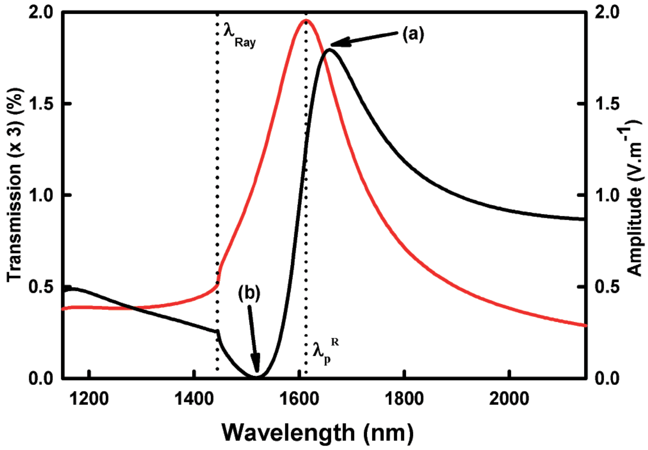
which gives a simple Lorentzian profile, related to a Breit-Wigner resonance (see for instance the red curve of Fig.5). As shown in Fig.5, for a given eigenmode (*i.e.* λ_p imposed), the value of λ for which I_{BR} is a maximum (*i.e.* $\lambda = \lambda_p^R$) does not correspond to the location of I_F maximum or minimum (*i.e.* (a) or (b) in Fig.5).

In order to illustrate the physical mechanisms responsible for the behaviour described by the scattering matrix formalism, we represent the corresponding processes involved.

In Fig. 6, circles A and B represent diffracting elements e.g., holes. So an incident homogeneous wave i (in red) diffracts in A and generates a nonhomogeneous diffraction order (blue dashed line). Such an order is coupled with an eigenmode, which is characterized by a complex wavelength λ_p. It then becomes possible to excite this eigenmode, which leads to a feedback reaction on the nonhomogeneous order (one can talk then about a resonant order). This process is related to the resonant term of the scattering matrix. In Fig.5, the red curve is the electromagnetic field amplitude calculated for such a nonhomogeneous resonant order. The resonant diffraction order •••



▲ **Fig. 4:** Diagrams of slab modes. The electrostatic potential V of modes is plotted as a function of the location in the slab. Above: antisymmetric and symmetric modes. Below: pure surface mode, with each interface decoupled from each other.



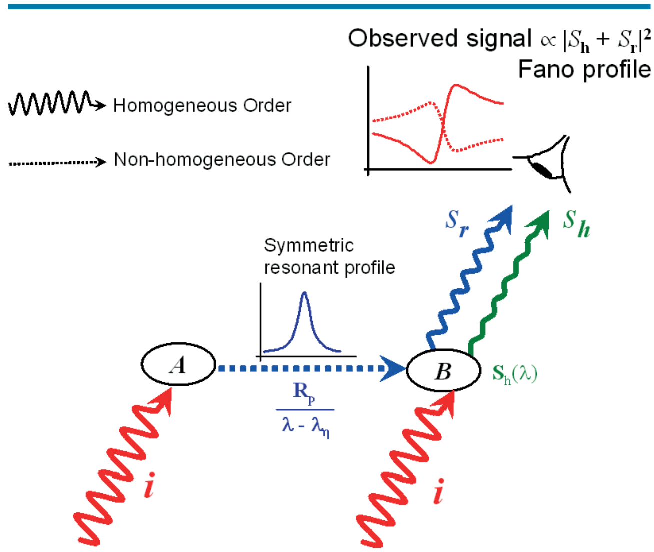
▲ **Fig. 5:** Computed optical transmission (black curve) and amplitude of the related resonant order (red curve) of a thin fictitious film (the permittivity is equal to $i1$) deposited on glass. 500 nm is set for the radius of each hole and the lattice parameter is taken to be a = 1000 nm. A discontinuity appears at the Rayleigh wavelength λ_{Ray}.

··· diffracts then in B, and generates a contribution to a homogenous diffraction order, in our case the specular beam. Thus one can ideally expect to observe a resonant profile, *i.e.* Lorentzian-like, for the amplitude s_r of the homogenous specular diffraction order that appears in B. Nevertheless, it is also necessary to account for nonresonant diffraction processes related to the holomorphic term $S_h(\lambda)$. So the incident wave i, generates also a homogeneous order S_h (in green), which appears as another contribution to the specular beam. So, as one observes the specular transmitted beam, one observes the sum of two rates, *i.e.* $s_r + s_h$. So, the Fano profiles of the transmission (but also of the reflection) result from a superposition of resonant and nonresonant contributions to the observed diffraction order [10-11]. As a result, in Fig.5 one can observe the calculated transmission (black curve) in comparison with the non-homogeneous resonant order amplitude (red curve).

Consequences and observations

As shown in Fig.3, the observed optical transmission through subwavelength hole arrays, exhibits a set of peaks and dips. Following the previously described approach, we have shown in recent works that the transmission spectrum is better depicted as a series of Fano profiles (see Fig.3 and Fig.5) [10,13,14]. These recognizable line shapes result from the interference of nonresonant transfers with resonant transfers, which involve the eigenmodes film, and evanescent diffraction orders. We could then point out that each transmission peak-dip pair is nothing other than a Fano profile. The appearance of an assymetric Fano line shape does not necessarily locate the peak or the dip at the eigenmode resonance (as shown in Fig.5), contrary to what has been suggested in some earlier works [7,8]. However, we have shown that the existence of the eigenmodes is a condition for the presence of the Fano line shapes. It can be noted that recent results by Genet et al confirm this description [11]. As a further outcome of this work it became clear that this kind of transmission spectrum, with its Fano line shapes, could also be obtained in a large context and that the generic concept of eigenmodes must substitute that of SPs only. These results implied two important ideas. First, according to the contributions of resonant and nonresonant processes in the Fano profile, eigenmodes can be associated with wavelengths closer to the peaks or to the dips. Second, it is possible to obtain transmission curves similar to those of metal films, by substituting SPs with guided modes or other types of polaritons. Many examples can be found, including highly refractive materials defining guided modes or ionic crystals in the restrahlen band defining phonon polaritons. For instance, we have reported simulations of a device, which consists of arrays of subwavelength cylindrical holes in a tungsten layer deposited on a glass substrate [13]. Tungsten becomes dielectric on a restricted domain of wavelength in the range 240–920 nm, *i.e.*, the real part of its permittivity becomes positive. So, whereas plasmons cannot exist, we show that the transmission pattern is similar to that obtained in the case of a metallic film. Indeed, it was also shown that in this case, instead of SPs, guided modes are excited [13]. Nevertheless, these modes give less intense fields than those achieved with SPs. In this way the benefit for the transmission is less important than with SPs modes. In the same way, it was also demonstrated that the transmission profile of a chromium film, in the restricted wavelength domain (1112–1292 nm), where the dielectric constant is positive, should involve eigenmodes, which are not SPs or guided modes. In this case, SPs can be substituted by Brewster-Zennek (BZ) modes [14]. Lastly it should be noted that in both cases, these theoretical computations are supported by experimental results.

As a consequence, it appears that bounded modes can act as a mediator of the optical transmission in bidimensional subwavelength hole arrays. Although it appears that the mechanisms involved in these devices have been implicitly known for a long time, it seemed important to us to recall it. Indeed, an important engine of the technological development is also the



▲ **Fig. 6:** Diagrammatic representation of the processes responsible for the behaviour of the transmission properties.

improvement of our theoretical knowledge of the phenomena with which we are confronted. ■

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Fun with the setting sun

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The setting sun plays a few tricks that any physicist will appreciate. One of these is well known: the sun appears unusually red when setting. It is the $1/\lambda^4$ dependence of Rayleigh scattering which selectively removes the blue end of the spectrum from the transmitted light.

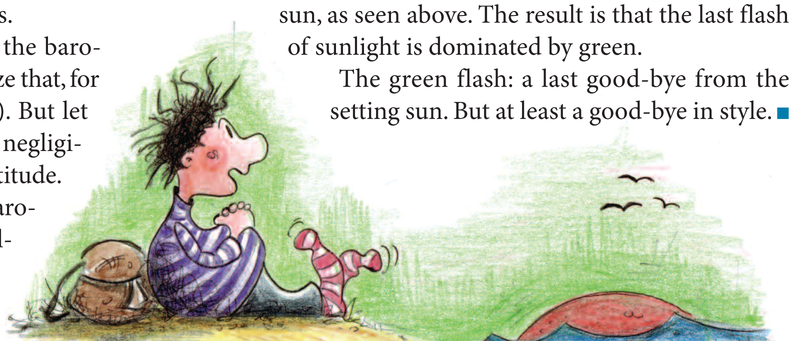
Less well-known is the fact that the sun is not where it seems to be, during sunset. In fact, it may be behind the horizon while we still see it. We are not talking here about the finite speed of light, which makes us see the sun about 8 minutes late. We are talking about the refraction of the sunlight due to the vertical gradient in the index of refraction, which in turn is caused by the density gradient. If we ignore temperature gradients for a second, the density decreases with height due to the decreasing atmospheric pressure, by a little over 1% for every 100 meter, *i.e.*, $n^{-1}(dn/dz) \approx 1\text{x}10^{-4}$. As a result, the light rays are bent downward, in the direction of the earth's curvature. This may be seen as the inverse of the well-known 'highway mirage', the apparent pools lying across the pavement when the sun shines.

Granted: temperature effects can be larger than the barometric pressure effects, which is easily seen if we realize that, for constant pressure, we have $n^{-1}(dn/dz) = -T^{-1}(dT/dz)$. But let us look at what happens if temperature gradients are negligible, or – even nicer – if temperature increases with altitude. Then the temperature effect – if any - adds to the barometric pressure effect. Now the light rays tend to follow the earth's curvature, which makes us see the sun just after sunset. This effect occurs both at sunrise and at sunset, and adds an extra 5 minutes of daylight to each day. Note that the finite-speed effect mentioned above does not do that; it just gives an 8-minute offset throughout the day.

Since bending of light rays in the atmosphere is stronger for lower-lying rays, there is a second phenomenon: the sun appears to be flattened by about 10%. The fact that we do not always notice this is due to the competing effect of temperature.

Finally, there is the somewhat mysterious 'green flash' that people sometimes observe at the moment of sunset. It lasts only for a few seconds, and requires somewhat favourable atmospheric conditions. Why green, and why only for a few seconds? There are a few things here that we have to combine. First the refraction, which makes us see sunlight after the actual sunset. Due to dispersion this effect is strongest for the blue end of the visible spectrum. This means that we expect blue to be visible longest, while the red end of the spectrum has long disappeared. But blue light is almost absent in the setting sun, as seen above. The result is that the last flash of sunlight is dominated by green.

The green flash: a last good-bye from the setting sun. But at least a good-bye in style. ■



A thermo-magnetic wheel [DOI: 10.1051/EPN:2007013]

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Who, in his childhood, was not astonished to see the linear momentum of a gentle breeze or a waterfall transformed to the angular momentum of a wheel? What wind and water have done for centuries, a thermal current can do today. A beam of absorbed radiation creates heat, a thermal current, which is directly and continuously transformed to a rotating wheel.

The development of high field magnets, such as those made of NdFeB (Neodymium-Iron-Boron) enables to use heat to rotate a wheel at room temperature. Such magnets, formed as small cylindrical discs, can be levitated in a magnetic dipole field [1,2]. If locally heated at the upper surface the levitated magnet starts to oscillate with increasing amplitude until it rotates like a wheel. It will do so as long as the heat flow is maintained. Radiation energy is transformed, at least partially, into rotational energy. The thermo-magnetic wheel is an example of self-exciting, oscillatory periodic motion that ends in a stable cycle limit, where there is a balance between energy input and dissipation [3]. The amazing effect is illustrated by a video, which can be obtained from the author upon request.

Experiment

The experimental setup is sketched in Fig. 1 and pictured in Fig. 2. The lifting magnets [B] are blocks or cylinders of NdFeB, axially magnetized, with maximal field strength of B=0.5 T at the surface and about 6 mT at the position of the floating magnet. The bismuth discs are cylindrical, approximately 30 mm in diameter and 13 mm in thickness. The geometry of these magnets and discs is not crucial. The floating magnet generates a maximal magnetic field of 0.5 T and is 8 mm in diameter, 3 mm thick, and weighs 1.2g.

Stable magnetic levitation is excluded by the well-known Earnshaw theorem [4]. However, by placing a diamagnetic material, such as bismuth, at the right position, a three-dimensional potential well is created. In this well, stable levitation in free space is possible. The small magnet is supported by carefully adjusting the lifting magnets so as to create a free-floating position between the bismuth plates.

What is seen?

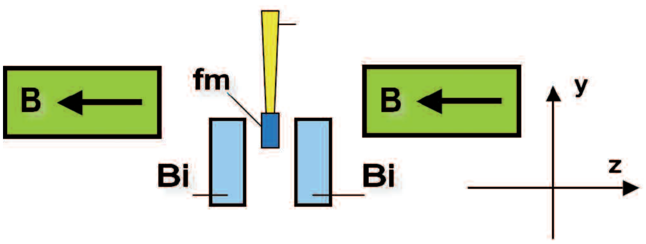
The motion of the magnet is recorded with both a video camera and a LASER beam. When the beam is reflected from a marked surface of the magnet, it hits a photocell. When the light is on, i.e. when a continuous heat input is present, motion starts from the equilibrium position, and the magnet behaves like a self-excited oscillator. The oscillation begins at an angular frequency $\omega(t)$ of about 2 rad/s. After several oscillations, $\omega(t)$ decreases to a minimum, due to the anharmonic motion at large angles. The motion then rapidly changes into a permanent steady-state rotation. Fig. 4 illustrates two typical examples of this motion.

A physical model

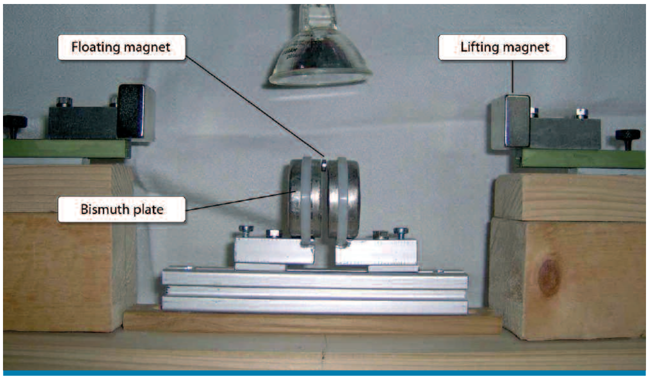
The thermo-magnetic wheel is modelled as a circular disc in harmonic rotational motion. The disc is suspended at a point, which we denote as magnetic suspension point [msp]. This point does not generally coincide with the centre of mass [cm]. Fig. 5 shows the system in the x-y plane normal to the z-axis.

The magnetic levitation force, which we denote by F_m, matches the weight F_w and has an action point, which lies higher than the gravitational centre of mass [cm]. The action point is not at [cm] because there are always slight inhomogeneities of the total magnetisation **M** with respect to the cylindrical geometry of the magnet. The magnet would be unstable in the z-axis direction without the Bi plates, and would quickly be pulled to one of the lifting magnets. With the diamagnetic bismuth plates, however, there are repulsive forces acting on the levitated magnet that obey an inverse 4th power law with distance, leading to a stable equilibrium position.

If gently displaced from its equilibrium position, the magnet will oscillate about the magnetic suspension point [msp] in both the x and y directions, horizontally and vertically. This means that the magnet is suspended in the magnetic field in



▲ **Fig. 1:** The parts of the system are: The lifting magnets [B], the bismuth discs [Bi], the floating magnet [fm] and a radiation beam [rb].



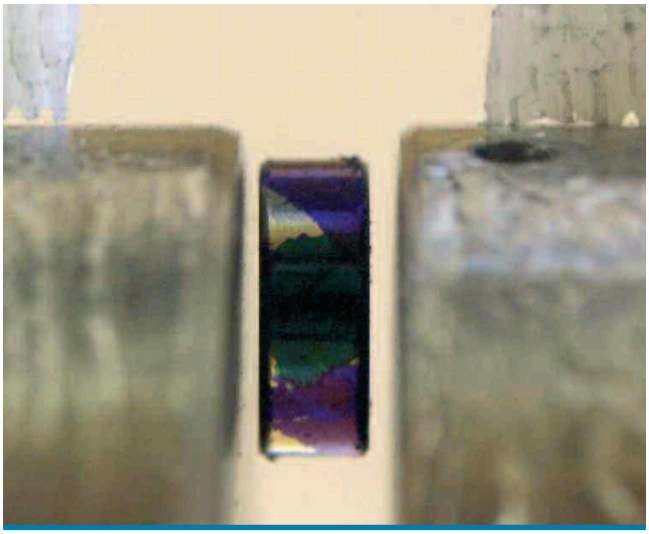
▲ **Fig. 2:** The lifting magnets are quadratic blocks, 25x25 mm and 12 mm thick. They can be moved on a track. The floating magnet lies between the bismuth plates and floats without touching them. A 12V spotlight is the radiation source.

every direction. Without radiation the magnetic suspension point is fixed. The motion is given by the differential equation for harmonic motion:

$$I\ddot{\phi} + R\dot{\phi} + D^*\phi = 0 \qquad (1)$$

where the $\dot{}$ stands for the time derivative, I is the moment of inertia, R the coefficient of the friction torque $R\dot{\phi}(t)$, and $D^* = m\,g\,D$, the coefficient of the restoring torque ($D^*\phi$), and D is the distance between the action points of the magnetic and gravitational forces. ϕ is the angle of rotation shown in Fig. 5.

We measured the natural angular frequency of the system to be $\omega_o = 2.1$ rad.s^{-1}, and we estimated a mean oscillation decay time to be approximately $\tau_{osc} = 50$s, so we can calculate all relevant oscillation parameters, R, D* and D. With $I = 9.6\ 10^{-9}$ kgm^2 we get: $D = \omega_o^2 I/mg = \omega_o^2 r^2/2g = 3.6\ 10^{-6}$m, $D^* = \omega_o^2 I = 4.2\ 10^{-8}$ Nm/rad, and $R = I/\tau_{osc.} = 1.9\ 10^{-10}$ Nms/rad, where m = 1.2g is the magnet's mass and g is the gravitational acceleration.



▲ **Fig. 3:** Magnified section of the floating NdFeB disc magnet between the diamagnetic bismuth plates. The levitated magnet is 8mm in diameter and 3 mm in thickness.

What is the reason for the self-excitation?

This thermo-magnetic wheel shows a startling behaviour when a heat flow is applied from above. The magnet starts to oscillate from rest with increasing amplitude. Some immediate questions are: Why does the amplitude of this oscillation increase? What is the source of the oscillation energy? What is the energy-transfer mechanism, and what is the equation of motion for the angular displacement ϕ between 0 and 2π?

Let us consider the equilibrium position for the disc magnet sketched in Fig. 6. The potential energy U of the floating magnet with a magnetic dipole moment **M** in the magnetic field **B** of the lifter magnet is [2]:

$$U = \mathbf{M.B} + mgy = -MB + mgy \qquad (2)$$

where mgy is the gravitational energy. In the absence of heat the floating magnet will align with the field **B**. There is no magnetic torque. The resulting net force $F_{net} = -\text{grad}\,U$ on the magnet is zero.

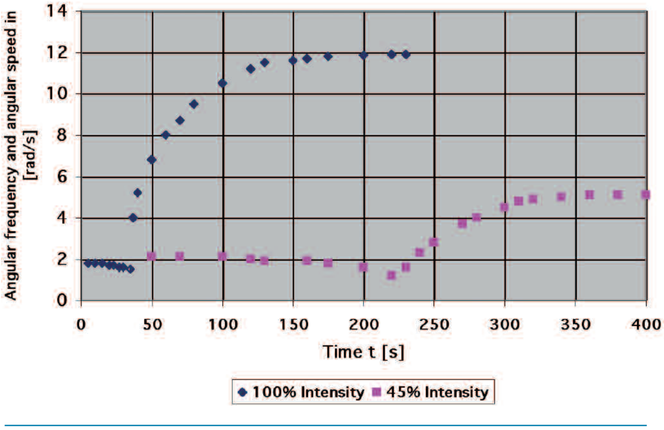
When the light is on, the upper magnet's surface is heated, and the local magnetisation decreases. Consequently the magnetic suspension point [msp] sinks gradually for about 1mm to a new equilibrium position inside the inhomogeneous lifting **B**-field. This shift of the [msp] generally leads to a misalignment of **M** and **B**, and a torque τ appears.

The heated region, which got a "thermal kick" at t = 0, moves away from the direct heat influx area and cools exponentially. Denoting the local magnetisation, i.e. the part of **M** which is affected by the thermal flow, as $\mathbf{M}_T$, we have: $\mathbf{M}_T = \mathbf{M}_o\exp(-t/t^*)$ [5]. The phenomenological constant t* describes the temperature decline of the magnetic dipole $\mathbf{M}_T$, as sketched in Fig. 6. $\mathbf{M}_o$ is the difference of the magnetic dipole between the initial and final states when the magnet rotates permanently, $\mathbf{M}_o = \mathbf{M}_{initial} - \mathbf{M}_{final}$.

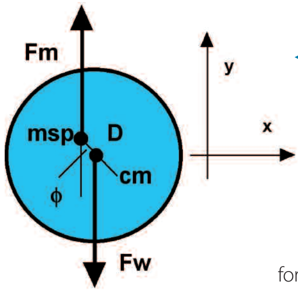
Since **M** and **B** are no longer aligned, a torque $\tau = \mathbf{M}_T \times \mathbf{B}$ acts on the magnet in addition to the gravitational one. This torque resembles the one observed in the gyro-magnetic experiment of Einstein and de Haas in 1915 [6]. There, the change in direction of the magnetic dipole **M** also causes a corresponding change in the angular momentum of a ferromagnet. Therefore there is a torque $\tau = \mathbf{M}_{Txy}\,\mathbf{B}_{xy}\sin(\phi)$ about the z-axis, where $\mathbf{M}_{Txy}$ and $\mathbf{B}_{xy}$ are the respective magnetic vectors in the x-y plane, and $\phi = t^*\dot{\phi}$ is the angle between them. We have

$$\tau = A\sin(t^*\dot{\phi}) \qquad (3)$$

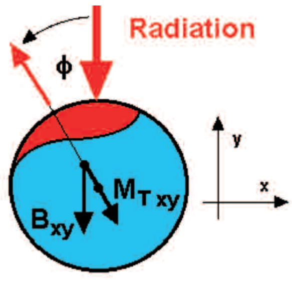
where A and t* are constants, chosen by best fit to the numerical solutions for the magnet's motion. The additional torque τ does not depend on time explicitly, but it acts on the pendulum ···



▲ **Fig. 4:** The angular frequency ω(t) is around 2 rad/s for the oscillation sequence. The angular speed ω(t) for the rotation is drawn as function of time for two heat intensities.



◀ **Fig. 5:** Levitated magnet as an oscillating disc. [D] is the distance between the centre of mass [cm] and the magnetic suspension point [msp] while ϕ denotes the rotational angle measured relative to the equilibrium axis defined by msp and cm. The z-axis is directed out of the XY plane. The static forces F_m and F_w are shown.



▶ **Fig. 6:** The magnet's position after receiving a "thermal kick" at t = 0 at the position ϕ = 0. The position angle ϕ is $t^*\dot{\phi}$, where t* is the time constant of the local exponential temperature decay. The magnetic dipole $\mathbf{M}_T$ and the levitating **B**-field are shown. The static forces $\mathbf{F}_m$ and $\mathbf{F}_w$ are omitted.

... just as the gravitational restoring torque does. If we add this torque to Equation (1) leaving, however, the small angle approximation, we get:

$$I\ddot{\phi}+R\dot{\phi}+D^*\sin(\phi)=A\sin(t^*\dot{\phi}) \qquad (4)$$

Equation (4) is a homogeneous, non-linear differential equation with no external independent function of time. We solve Equation (4) by numerical approximation using MATHEMATICA with the numerical values $\omega_o^2 = D^*/I = 4.4$ [s^{-2}], ϕ[0]=0, $\dot{\phi}$[0] = 0.2 [s^{-1}], R/I= 0.02 [s^{-1}], A/I = 0.9 [s^{-2}] and t*= 0.25 [s]:

$$\ddot{\phi}+0.02\dot{\phi}+4.4\sin(\phi)=0.9\sin(0.25\dot{\phi}) \qquad (5)$$

In Fig. 7 we plot the angular velocity $\omega(t) = \dot{\phi}(t)$ obtained after numerical differentiation of $\phi(t)$. The angular displacement $\phi(t)$ is the numerical solution of equation (5). Fig. 7 is a quantitative correct picture of the observed self-excited oscillation and subsequent rotation. An oscillation is superposed on the rotation; it is due to the slight eccentricity of the thermo-magnetic wheel. Also, equation (5) gives solutions for the cases when light does not hit the magnet vertically, but is displaced by $\pi/2$ or π, i.e. when $\phi_{torque} = \phi$ +/-$\pi/2$ or $\phi_{torque} = \phi + \pi$; these cases are experimentally confirmed. This mechanism of self-excitation by a continuous thermal flow resembles very much the wind-driven oscillations observed in 1940 at the Tacoma Narrows bridge in the USA [7].

After the transient self-excited oscillations end, the magnet continues in rotation with a constant mean angular speed $\omega(t)$. The temperature of the magnet reaches a constant value, T^∞, and the thermal gradient goes away. A new, dynamically stable state is reached. The active magneto caloric forces, which initiated the oscillation, become a small torque. This torque matches the minute external torque due to air drag and, perhaps, eddy current dissipation.

Is the thermo-magnetic wheel a heat engine?

Yes, because this simple room temperature experiment transforms radiation heat directly to rotational motion of a wheel. This amazing effect can be described completely within the framework of a thermo-magnetic self-excitation mechanism. The thermal flow through the levitated magnet provides energy to sustain the oscillation and subsequent rotation. However, its potential as a source of mechanical power is presently not very attractive. A rotating magnetic field is, in principle, a Faraday disc generator. We estimate the heat energy flowing per second through the magnet to be around 10 mJ, while the rotating energy of the magnet is less than 1μJ. This minute rotational energy cannot compete with solar-based energy converters.

This analysis describes an angular pendulum that transfers energy between radiation-, magnetic- and gravitational fields. The model adequately explains the observations. This thermally driven "heat wheel" combines gravity, magnetism and electromagnetism, as well as thermodynamics and mechanics, in a simple demonstration that is unique and unusual. ■

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Claudio Palmy received his Ph.D. in superconductivity from the Swiss Federal Institute of Technology Zürich, ETHZ, in 1970. After a short time as a visiting professor in Sao Paulo, Brasil, he became a physics professor at NTB, Interstate University of Applied Sciences of Technology Buchs, Switzerland. Since 2004 he has worked on magnetism at the Alpine Institute of Physics Stuls, Switzerland. E-mail: cpalmy@bluewin.ch

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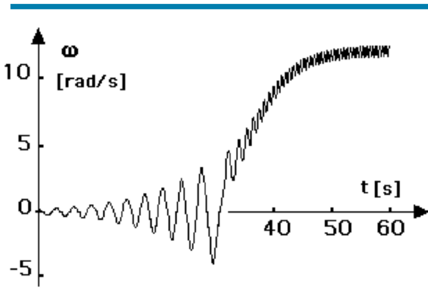

◀ **Fig. 7:** Calculated angular velocity $\dot{\phi}$ (t) = ω(t) for a levitated magnet in a vertical (y-axis) temperature gradient at room temperature.