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Editorial

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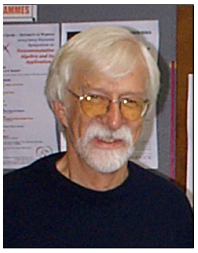

The 15th anniversary the ESI in April 2008 was an occasion not only for celebration, but also for an evaluation of the Institute's performance over the past 5 years and its scope for future development.

The previous evaluation of the ESI in 2003 had been chaired by Nigel Hitchin (Oxford), who had recruited as co-evaluators Robbert Dijkgraaf (Amsterdam), Jürgen Jost (Leipzig), Nicolai Reshetikhin (Berkeley) and Vincent Rivasseau (Orsay).

The evaluation in 2008 followed essentially the same pattern: Peter Goddard (IAS Princeton) agreed to chair the evaluation and chose for his panel of co-evaluators Jean-Michel Bismut (Orsay), Robbert Dijkgraaf (Amsterdam), Felix Otto (Bonn) and Scott Sheffield (Courant Institute). After a site visit by the panel in April 2008 the final report of the evaluation was sent to the Austrian Ministry of Science in June 2008.

Apart from praising the quality of the programmes which had taken place at the ESI during the past five years, he review panel noted that the Institute had 'gently and wisely' increased its scope of the programmes in recent years, into areas of pure mathematics more remote at present from theoretical physics, and into areas of physics and biology beyond those usually characterized as mathematical physics. The panel felt that this process should be continued in the same judicious fashion as in recent years.

The report also contains a number of recommendations for the development of the ESI over the next years. These proposals and their financial implications are currently under further discussion with the University of Vienna and the Austrian Ministry of Science.

On behalf of the Erwin Schrödinger Institute I would like to send seasons greetings and my best wishes for a happy and peaceful year 2009.

EVALUATION OF THE ESI, APRIL 2008

The scientific directors of the ESI, **Joachim Schwermer** and **Jakob Yngvason**, together with the evaluators **Peter Goddard** (IAS Princeton, chair), **Scott Sheffield** (Courant Institute), **Jean-Michel Bismut** (Orsay) and **Felix Otto** (Bonn) – from left to right.

Nobel Prize in Physics 2008: Symmetry Violation in Subatomic Physics

Gerhard Ecker and Walter Grimus

The Nobel Prize in Physics 2008 was awarded to Yoichiro Nambu (Enrico Fermi Institute, Chicago, USA) for "the discovery of the mechanism of spontaneous broken symmetry in subatomic physics" and to Makoto Kobayashi (KEK, Tsukuba, Japan) and Toshihide Maskawa (Yukawa Institute for Theoretical Physics, Kyoto, Japan) for "the discovery of the origin of the broken symmetry which predicts the existence of at least three families of quarks in nature."

Symmetries in physics

The modern view of symmetries as groups of transformations that leave the equations of motion invariant emerges in the 19^{th} century. With the advent of quantum mechanics in the 1920s, symmetries were found to explain degeneracies in spectra and to give rise to relations between measurable quantities such as cross sections and decay rates. In addition to the classical space-time symmetries (Galilei, Poincaré), a new type of symmetries occurs in quantum field theories: the so-called "internal" symmetries do not affect space and time but they transform the fields of the theory. The gauge symmetries of the fundamental interactions are prominent examples.

Symmetries play an important role in subatomic physics:

i. Unlike gravitational and electromagnetic forces, nuclear forces are remote from our everyday experience. From the study of spectra and other observables, physicists extract clues for underlying symmetries to be implemented in the corresponding quantum field theories.

ii. Theoretical physics often proceeds by analogies and extrapolations: extending the gauge symmetry of the electromagnetic interaction to the weak and strong interactions led to the modern theory of the fundamental interactions, the Standard Model (SM) of particle physics.

Till the middle of the last century, symmetry principles were thought to express the basic simplicity of nature. The discovery that some of the "sacred" symmetries such as parity (P), time reversal or charge conjugation (C) were only approximate came therefore as a surprise. In his Nobel Lectures of 1979 Weinberg expressed this feeling as a question: "Is nature only approximately simple?" By now there is a general consensus that also approximate symmetries may reveal fundamental properties of nature. For instance, CP violation is essential for the baryon asymmetry of the universe and thus for our existence [1].

Symmetries in particle physics can be classified in four groups:

1. Exact symmetries leave the field equations and the ground state of the theory invariant. Examples are the Poincaré transformations (Lorentz transformations and space-time translations) and the gauge symmetries of electromagnetic and strong interactions.

2. Spontaneously broken symmetries still leave the field equations invariant, but not the ground state. Nambu was the first to realize the importance of this concept in relativistic quantum field theories. Examples are the chiral symmetry of the strong interactions (in the limit of vanishing quark masses) and the electroweak gauge symmetry.

3. Approximate symmetries do not even leave the field equations invariant, but traces of the symmetries are still visible in measurable quantities. Symmetries violated only by the weak interactions (P, CP, strangeness, ...) are of this type. Kobayashi and Maskawa received the Nobel Prize for their explanation of CP violation in the SM.

4. Anomalous symmetries leave the classical field equations invariant, but are violated by quantum effects.

Spontaneous symmetry breaking

The notion of spontaneous symmetry breaking originated in solid state physics. For example, the Hamiltonian describing a ferromagnet is rotationally invariant in the absence of an external magnetic field, yet the ground state exhibits spontaneous magnetization along some arbitrary direction: rotational symmetry is spontaneously broken in the ferromagnet.

The main inspiration for Nambu came from the BCS theory of superconductivity [2]. In certain metals, the electron-phonon interaction can lead to the formation of Cooper pairs (two electrons with opposite momenta and spins) that condense in the ground state. The ground state is therefore charged implying the spontaneous violation of gauge invariance. In an important paper [3], Nambu demonstrated that gauge invariance, although not manifest in the BCS theory, is nevertheless fully maintained.

That was the starting point for Nambu and Jona-Lasinio to investigate the structure of the ground state in relativistic quantum field theories relevant for particle physics. The Lagrangian of the Nambu–Jona-Lasinio (NJL) model [4]

$$\mathcal{L}_{\text{NJL}} = \overline{\psi}\gamma^\mu i\partial_\mu\psi + g_0\left[\overline{\psi}\psi\overline{\psi}\psi - \overline{\psi}\gamma_5\psi\overline{\psi}\gamma_5\psi\right]$$

describes the self-interaction of a single nucleon field ψ and is modeled after the BCS Lagrangian. Because of the absence of a mass term $m_\psi\overline{\psi}\psi$ the Lagrangian and the field equations are invariant with respect to two independent phase transformations (chiral symmetry)

$$\psi(x) \to e^{i\alpha}\psi(x), \quad \psi(x) \to e^{i\beta\gamma_5}\psi(x)\,.$$

Depending on the size of the coupling constant g_0, the ground state of the theory may exhibit spontaneous breakdown of the chiral symmetry, generating both a finite mass for the initially massless nucleon and a massless collective excitation (pion). The modern version of the NJL model is Quantum Chromodynamics (QCD), the gauge theory of quarks and gluons for the strong interaction. Chiral symmetry holds for massless quarks, which is a good approximation for the two lightest quarks u, d. Spontaneous breaking of chiral symmetry provides the only plausible explanation why pions are by far the lightest hadrons.

In the NJL model, most of the nucleon mass arises from spontaneous chiral symmetry breaking. According to our present understanding, the small u and d masses contribute actually only about 5% to the nucleon mass. In other words, 95% of our mass and of the visible universe are due to the strong quark-gluon interaction in QCD. Only the small remainder requires a different mechanism for mass generation.

Inspired by the work of Nambu and Jona-Lasinio, Goldstone demonstrated [5] that spontaneously broken symmetries lead to

massless excitations in general. In the case of so-called global symmetries (e.g., chiral symmetries), these excitations would be massless particles (pions for $m_u = m_d = 0$). As shown a few years later by Brout and Englert [6] and by Higgs [7], the situation is different for gauge symmetries (local symmetries): the Nambu-Goldstone excitations are not physical particles but they render some of the initially massless gauge vector fields massive. This is the relativistic analogue of the Meissner effect in superconductivity. In particle physics, it is known as the Higgs effect of spontaneous gauge symmetry breaking.

Based on the foundations laid by Nambu, spontaneous symmetry breaking is an established phenomenon in the SM. Spontaneous breaking of the electroweak gauge symmetry is responsible for the masses of W and Z bosons, the carriers of the weak interactions, and for the masses of quarks and charged leptons. However, the specific implementation of this mechanism remains to be uncovered. It was one of the main motivations for building the collider LHC at CERN to unravel this mechanism. The Higgs model of spontaneous gauge symmetry breaking describes only one of the possible scenarios.

The original work of Nambu was concerned with the strong interaction. His discoveries paved the way for the formulation of an effective quantum field theory of hadrons at low energies ($E \ll 1$ GeV) where the usual perturbative treatment of QCD cannot be applied because of the permanent binding of quarks and gluons (confinement). In the words of the Nobel Committee, this effective field theory called Chiral Perturbation Theory has become the "... standard tool to compute strong interaction processes in this energy range ..." The Particle Physics group at the University of Vienna has provided and applied some of those tools during the past 20 years.

Explicit breaking of the CP symmetry

In the second half of the fifties, inconsistencies in the interpretation of weak-decay data became a pressing problem. In 1956, in a beautiful theoretical paper, Lee and Yang proposed P violation in weak interactions as a resolution to this problem and suggested to test this hypothesis in β-decay of polarized nuclei or particles. Soon thereafter, P violation was confirmed in the decay of ^{60}Co and, nearly simultaneously, in muon decay. The successful conclusion of this fundamental issue was provided by the V–A (vector minus axial vector current) theory of weak interactions in which both P and C are maximally violated.

In the V–A theory, CP was conserved in a natural way. Therefore, the discovery of the decay $K_L \to \pi^+\pi^-$ in 1964 at the Brookhaven National Laboratory [8], a manifestation of CP violation, was completely unanticipated and provided a new puzzlement which did not diminish with the advent of the SM of electroweak interactions, in which the V–A theory found a home as a certain low-energy limit.

The SM was formulated with leptons and quarks. To account for the hadrons known at that time, three quarks u, d and s were sufficient. The mixing between d and s—the famous Cabibbo angle—could straightforwardly be transferred from pre-quark models [9] to the SM. However, apart from the CP problem, another unexplained experimental fact remained, namely the absence of flavour-changing neutral currents at the tree level, manifesting itself in the severe suppression of decays like $K^+ \to \pi^+ e^+ e^-$. This problem was solved in 1970, when Glashow, Iliopoulos and Maiani proposed the existence of a fourth quark, the charm quark c, which provided a very simple mechanism to remove flavour-changing neutral currents, the so-called GIM mechanism [10].

This was the situation when Kobayashi and Maskawa, at that time both at Kyoto University, wrote their famous paper [11]. Although the c quark was discovered only in 1974, they took the "quartet scheme", i.e. the existence of four quarks, for granted. The bulk of the paper consists of the proof that for all possible assignments of the four left-handed and the four right-handed quark fields to multiplets of the SM gauge group $SU(2) \times U(1)$, CP violation was either absent or, if present, there was a contradiction to experiment. Thus they concluded that "no realistic models of CP violation exist in the quartet scheme without introducing new fields." One of their suggestions for new fields was a second Higgs doublet, an extension of the SM that is still investigated today. Nearly at the very end of the paper they suggested the introduction of a third family of quarks, a courageous venture at a time when not even the fourth quark had been discovered, which eventually earned them the Nobel Prize.

Why is the number of quark families connected with CP violation? The point is that CP violation is caused by complex coupling constants in the interaction Hamiltonian. The weak charged-current interaction Hamiltonian density is given by

$$\mathcal{H}_{cc} = \frac{g}{2\sqrt{2}} \left(\bar{\mathbf{u}} \gamma^\mu (\mathbb{1} - \gamma_5) V \mathbf{d}\, W_\mu^+ + \text{H.c.} \right),$$

where W^+ is the W-boson field, g is the $SU(2)$ gauge coupling constant and $\mathbf{u}$ and $\mathbf{d}$ are the column vectors containing the quark fields with charge $2/3$ and $-1/3$, respectively. In $\mathcal{H}_{cc}$, the quark fields are assumed to be mass eigenfields. The matrix V, nowadays called Cabibbo–Kobayashi–Maskawa or CKM matrix, appears as a consequence of the diagonalization of the complex mass matrices for the quarks of both charges. It is a general $n \times n$ unitary matrix, where n is the number of quark families. It is an easy mathematical task to show that, if one absorbs $2n - 1$ phases into the fields $\mathbf{u}$ and $\mathbf{d}$, then the number of phases left over in V is $(n-1)(n-2)/2$. These phases are physical and their number is zero for one or two quark families. However, for $n = 3$ there is exactly one phase which produces CP violation; this is the important observation made by Kobayashi and Maskawa. The discovery of the bottom quark in 1977 as a member of a third quark family promoted the Kobayashi–Maskawa mechanism to a respectable and realistic candidate for the description of CP violation. The existence of the second member of the third quark family, the top quark, was established much later in 1995.

Until the year 2000, our knowledge about CP violation came exclusively from the $K^0 \bar{K}^0$ system. Only after 2000, with the advent of the results of the Belle experiment in Tsukuba, Japan, and of the BABAR experiment in Stanford, U.S.A., plenty of CP-violating observables were measured in B-meson systems, and the Kobayashi–Maskawa theory of CP violation was confirmed in a spectacular way.

One could ask oneself why CP violation is so elusive. This is intimately connected with the small mixing angles in V. Actually, using the fact that different columns of V are orthogonal, one can write down relations like

$$V_{ud} V_{ub}^* + V_{cd} V_{cb}^* + V_{td} V_{tb}^* = 0.$$

The three terms in this sum form a triangle in the complex plane. All such "unitarity triangles" that can be obtained from V have the same area. This area is a measure for the strength of CP-violating effects. The small quark-mixing angles imply a small area of approximately 1.5×10^{-5}, of the order of the sixth power of the sine of the Cabibbo angle [12]. Therefore, CP-violating effects are suppressed despite a

large CP-violating phase. In that sense, CP is an approximate symmetry even of the weak interactions. In other words, if CP violation in a process is large, then the process is rare; if a process is not rare, then CP violation is suppressed in this process.

The Kobayashi–Maskawa theory of CP violation is a stunning success story and will most probably experience further confirmation by future measurements. On the other hand, this mechanism of CP violation will have its limitations just as the SM with which it is inseparably connected. One limitation is already known: in order to explain the baryon asymmetry of the universe, the Kobayashi–Maskawa mechanism is not sufficient. Such an explanation requires an extension of the SM with new sources of CP violation.

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Metastability and Rare Events in Complex Systems

Christoph Dellago

Since its invention in the 1950s, molecular dynamics simulation has developed into a powerful and versatile tool in the physical sciences. Today, running on modern computers, molecular dynamics simulations are used to study the structure and dynamics of complex systems consisting of up to a few million atoms of interest in physics, materials science, chemistry and biology. In this method, the motion of individual atoms is followed in time by integrating the classical equations of motion for small time steps with forces obtained from empirical interaction potentials or *ab initio* by solving the electronic structure problem. By iterating this basic step, the time evolution can be determined, in principle, for arbitrarily long time. But in spite of the rapid growth in raw computing speed and impressive algorithmic advances, numerous processes occurring in nature and technology are still beyond the reach of current technology.

One of the factors that limits the practical applicability of molecular dynamics simulation is that many processes, such as the folding of a protein or the transport of a dopant through a semiconductor, are characterized by widely different time scales. Consider, for instance, the freezing of supercooled water. The fastest motions that need to be taken into account in a molecular dynamics simulation of this process are bond vibrations and molecular librations with periods of tens of femtoseconds as well as molecular reorientation taking place on the picosecond scale. To faithfully reproduce these rapid motions, time steps in the femtosecond range are necessary. In contrast, the time scale for the crystallization event is many orders of magnitude larger. It has been known for a long time that a sample of water, carefully cooled below the freezing point, can remain in the metastable liquid state for hours if not days, and only an external perturbation initiates the freezing process that turns the liquid into the thermodynamically stable crystalline phase.

The reason for this behavior is that freezing proceeds through the formation of a critical nucleus involving the creation of an interface between the crystallite and the metastable liquid phase. Due to the free energetic cost associated with the the interface, the process is uphill initially leading to a free energy barrier that opposes rapid solidification. Only once the crystalline nucleus grows beyond the critical size due to a rare statistical fluctuation, does the volume term in the free energy prevail and the phase transition occurs. Naturally, such long nucleation times, which can exceed the basic timescale of molecular motion by many orders of magnitude, present an enormous challenge for the computer simulator who attempts to study the freezing of water with molecular dynamics simulation. The number of steps required to observe one single event simply lies far beyond the possibilities of current (and future) computer systems. Similar complications arise in all systems in which energy barriers or entropic bottlenecks hinder the motion of the system and partition phase space into metastable basins. The dynamics of such systems is then characterized by infrequent but rapid transitions between long-lived states: we speak about rare events.

An important concept to deal with rare events is transition state theory, developed in the context of chemical kinetics by Eyring, Polanyi and Wigner [1, 2, 3] in the 1930s, long before the advent of fast electronic computers. The central idea of transition state theory is that during transitions between stable states separated by a high energy barrier, the system passes through a saddle point in the potential energy surface. This so called transition state provides the lowest energy passageway connecting the stable states located at potential energy minima. From the properties of the transition state one can then calculate reaction rates and glean information on the microscopic transition mechanism. In complex condensed phase systems, however, this simple picture on which transition state theory is based breaks down. In a condensed phase environment, stable states typically cease to be associated with individual minima in the potential energy surface. Rather, they can encompass a large

number of local minima and saddle points (the supercooled liquid from above, for instance, is certainly a long-lived metastable state but does not correspond to a particular potential energy minimum). Similarly, transition states can no longer be pictured as individual saddle points. This situation is depicted in Fig.1 which represents an artist's view of the potential energy surface in a complex high-dimensional system.

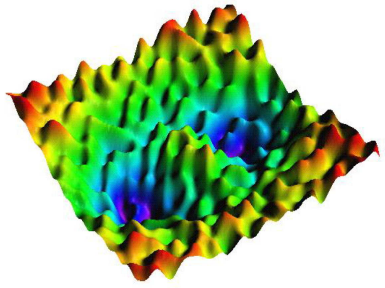

Figure 1: Low-dimensional caricature of a high-dimensional potential energy surface with multiple stationary point. Two deep stable states, containing several local minima and saddle points, are separated by a rugged free energy barrier.

In studying processes occurring on such energy landscapes a number of non-trivial questions arise that go beyond a mere time scale problem in the molecular dynamics simulation. How, for instance, can the long-lived states be identified in terms of the microscopic phase space coordinates? Which variables can be used to describe the transition and serve as a reaction coordinate? What are the transition states? How often do transitions occur? In the past couple of years several computational tools to simulate processes involving rare but important events and address such questions have been put forward. These new approaches and related issues were the focus of the ESI-program on *Metastability and Rare Events in Complex Systems*, February-April 2008, organized by C. Dellago, P. G. Bolhuis, and E. Vanden-Eijnden and attended by most of the researchers active in this field. One of the main goals of this workshop was to bring together people working on rare events in different areas ranging from physics and chemistry to materials science and molecular biology. In particular, the hope was to involve mathematicians and to establish closer links between researchers engaged in methods development and those working on large scale applications. In the following, I will briefly (and incompletely) survey a few of the key ideas and concepts discussed during the program. For a more thorough discussion of new developments in this area, I refer the reader to a recent review article [4].

Exploring configuration space

Configuration space is a big place. To explore all of its important regions is a challenging task, particularly if sampling is complicated by the presence of widely disparate time scales. One strategy to reduce the complexity of the problem is to introduce a small set of collective variables which are presumed to include all degrees of freedom that are important for the process of interest and cannot be replaced by random noise. The free energy landscape, determined as a function of these collective variables, then provides the information necessary to locate stable regions and identify possible routes for transitions between them. Of course, such a simplified picture obtained by integrating out most degrees of freedom is accurate only if the right collective variables have been chosen, an often exceedingly difficult problem.

While several computational methods such as umbrella sampling [5] or thermodynamic integration [6] for the computation of free energies as a function of one or two variables have been available for quite some time, only recently it has become possible to compute free energies in higher dimensions. The turning point came with the invention of the metadynamics method by Laio and Parrinello in 2002 [7]. The simple and effective basic idea of this method is to run molecular dynamics on a biased energy landscape. The bias is built up on the fly in a way to force the system to explore phase space regions it has not visited before. This is achieved by leaving behind repulsive Gaussian potentials acting on the preselected collective variables. These potentials effectively mark the already visited regions and drive the system into unexplored territory. As a result, one obtains possible transitions routes to other stable states and, as a bonus, the free energy as a function of the collective variables. The bias, however, perturbs the natural dynamics of the system such that dynamical quantities, *e.g.*, transition rate constants, cannot be computed with metadynamics. To date, metadynamics has been successfully applied to study numerous processes occurring in condensed phases including structural phase transitions in solids, chemical reactions, and biomolecular isomerizations.

Finding rare transition pathways

In a molecular dynamics simulation one specifies initial conditions and then lets the system evolve freely according to the underlying equations of motion. The system then explores configuration space without external guidance and often things happen serendipitously that could not have been easily anticipated. In the metadynamics method, one tries to accelerate this natural time evolution by preventing the system from returning to configuration space regions that have been sampled before. As in conventional molecular dynamics, the dynamics starts from given initial conditions and the state the system evolves to is not specified in advance: both approaches are single-ended methods.

In some situations, however, both the initial and the final state of a certain process are known, but not the mechanism that transports the system from one to the other. Think, for instance, of the crystallization of supercooled water considered above. Both the supercooled liquid as well as the ice crystal are well known and characterized, the detailed freezing mechanism on an atomistic scale, however, is still uncertain. Similarly, in many structural phase transitions occurring in solids, one exactly knows the stable and metastable phases, but has only vague ideas about the atomistic transition mechanism. In the past couple of years, some advances have been made in the development of double-ended path based methods designed to address this problem of rare transitions between known long-lived states.

One approach that has been applied to a large variety of rare event problems is transition path sampling, mainly developed by Dellago, Bolhuis and Chandler [8, 9]. The conceptual foundation of transition path sampling is the statistical definition of the set of all dynamical pathways that start and end in given regions of configuration space. This set of pathways, the transition path ensemble, is then sampled with a Metropolis Monte Carlo algorithm. The basic step of this procedure consists in generating a new path from an old one, for instance by shooting off the new trajectory from a point on the old one with slightly perturbed momenta. Then, the new path is accepted or rejected according to a criterion that satisfies detailed balance, thus guaranteeing that the desired path ensemble is sampled. Iteration of this step generates a biased random walk in the space of trajectories, in which pathways are visited according to their statistical weight in the transition path ensemble.

While the transition path sampling procedure contains a random element, individual pathways are fully dynamical trajectories governed by the deterministic or stochastic equations of motion of the system. Therefore, pathways harvested with transition path sampling can be analyzed to yield the mechanism as well as the kinetics of the transition. Since only reactive pathways are considered and typically rare barrier crossing events occur rapidly once they happen, no computing power is wasted to follow the time evolution during the uneventful permanence in the stable states. Current research efforts are directed towards the development of more efficient transition path sampling algorithms for the computation of rate constants and the ergodic sampling of pathways in systems with multiple transition routes. To date, the transition path sampling methodology has been used to study to a wide variety of processes in physics, materials science, chemistry, and biology. Applications range from first order phase transitions to chemical reactions in solution and biomolecular conformational changes. The transition path sampling method, including applications, is reviewed in [4].

Another recent approach to study transitions between known stable states discussed during the program at the ESI is the string method developed by E, Ren, and Vanden-Eijnden [10]. In this method, suitable for systems evolving according to stochastic dynamics and rooted in transition path theory [11], a string with endpoints anchored in the stable states is adapted iteratively according to an appropriate protocol until convergence is reached. The converged string can be viewed as a typical representative of high likelihood trajectories connecting the stable states, from which rates and mechanism can be extracted.

Identifying mechanisms

Transition path sampling and other methods for the simulation of rare events typically yield many realizations of the transition event. Further analysis is most often required to identify the exact transition mechanism in terms of a reaction coordinate, *i.e.*, a variable that quantifies the progress of the transition. Sometimes, watching the motion of individual atoms with a molecular viewing program on a computer can provide valuable insight and assist one's imagination, but too often this exercise is a sobering experience as the important degrees of freedom capturing the essential physics of the process remain elusive. Here, statistical analysis tools developed recently help to make progress.

The central concept, on which most of these algorithms build, is the committor, an idea going back at least to Onsager, who used it to analyze the dissociation of ions in solution [12]. This quantity, defined for a particular configuration, measures the probability that dynamical trajectories initiated from that configuration relax into one of the stable states rather than the other. The committor is the ideal reaction coordinate in the sense that it quantifies how far a reaction has proceeded and what is likely to happen next. While configurations near the stable states typically have committors close to 0 or 1, configurations with a committor of 1/2 located on top of the (unknown) free energy barrier can be viewed as transition states. These are states from which both stable states are equally accessible. With this statistical generalization of the concept of the transition state, an ensemble of transition states can be determined from which information on the transition mechanism can be inferred.

While the committor is, in a sense, the perfect reaction coordinate, it is very unspecific and it does not directly lead to a true physical understanding of the transition mechanism. The committor is, however, very useful for testing the quality of a postulated reaction coordinate [13]. While a good reaction coordinate parametrizes the committor, no such relation exists for a poor reaction coordinate. This idea is exploited in two computational methods for the automatic identification of reaction coordinates, based on genetic neural networks [14] and likelihood maximization [15]. There is no doubt that these and similar analysis methods will play a major role in future studies of rare event processes.

Outlook

The computational techniques and theoretical concepts briefly presented here and discussed at length during the ESI-program have been available only for a couple of years. Nevertheless, they have already contributed significantly to our understanding of many processes in complex condensed matter systems. In the future, one important challenge will be to combine the complementary strengths of these methods in order to efficiently cross the vast time-scale gap that lies between the macroscopic and the microscopic world. Hopefully, the ESI-program on *Metastability and Rare Events in Complex Systems* has helped to create new momentum and interactions for concerted efforts in this direction.

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Josef Stefan, Josef Loschmidt and Stigler's Law

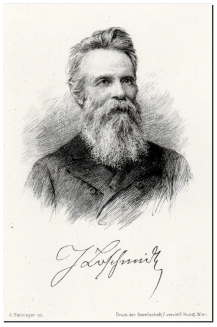
John Crepeau

Josef Stefan[1] and Josef Loschmidt[2] were both affiliated with the Institute of Physics at the University of Vienna in the latter half of the 1800s; Stefan as Director and Loschmidt as a researcher. Both came from poor rural families in the Austro-Hungarian empire, both made seminal contributions to science, but both have been recognized differently within the scientific community. Stefan's name[3] is associated with constants, physical laws and dimensionless numbers, while Loschmidt[4] has remained virtually anonymous, his contributions usurped by others.

Stigler's Law of Eponymy[5] states, "No scientific discovery is named after its original discoverer." This sociological observation shows that throughout the history of science, many who have made outstanding contributions are often not rightfully recognized. Among the great contributions made by Josef Loschmidt, two stand out as applications of Stigler's Law. After working in the chemical industry for a number of years, he longed to perform research, but was unable to gain a suitable position. So, he became a schoolteacher with the added perk that the school provide a small laboratory in which to do work in his spare time. Under these difficult circumstances, Loschmidt published, at his own expense, a booklet entitled *Chemische Studien I*[6], [7] (no part II ever appeared), where he diagrammed single, double and triple chemical bonds, as well as a novel way to construct a benzene molecule. Loschmidt hypothesized that the six carbon atoms be connected in a ring with one hydrogen atom be attached to each of the six carbon atoms. Since there was no experimental evidence to confirm this structure, his discovery was largely ignored and forgotten, except by one August Kekulé. Four years after reading Loschmidt's booklet, Kekulé proposed the same shape. This inspiration supposedly came to Kekulé after having a dream where he saw snakes grabbing on to their own tails, then whirling around in a circle. Today, it is very common to hear about Kekulé's dream and his "discovery" of the structure of the benzene molecule.

Stefan recognized Loschmidt's brilliance and subsequently hired him as a researcher at the Institute. While at there, Loschmidt became interested in James Clerk Maxwell's kinetic theory of gases. He figured that one way to calculate the size of a molecule would be to measure the density of liquefied gas, and assume that the molecules in liquid form were tightly packed together, occupying a volume only slightly larger than the volume occupied by the molecules themselves. From this basis, he used the kinetic gas equations developed by Maxwell and Rudolf Clausius to successfully calculate the size of a molecule. Maxwell himself used Loschmidt's methods to calculate the size of gas molecules in order to determine the diffusion coefficients of various gases.

Maxwell stated, "Loschmidt, in 1865, made the first estimate of the diameter of a molecule", and then used Loschmidt's values to calculate that, "in a cubic centimeter of gas at standard pressure and temperature there are about nineteen million million million molecules".[8]



Ludwig Boltzmann, a student both of Stefan and Loschmidt, first proposed that the number of particles in a cubic centimeter be called Loschmidt's number,[9] stating this was Loschmidt's greatest accomplishment. Despite Maxwell's and Boltzmann's explicit acknowledgement that Loschmidt provided the means of determining the number of atoms in a given volume, the name associated with this number (actually a close relative of the number) is Avogadro, who merely postulated that a given volume of gas is proportional to the number of atoms or molecules. Usage of the Loschmidt number is limited to German speaking countries. Poor Loschmidt never seemed to receive the credit he rightly deserves.

The name of Loschmidt's colleague, Stefan, appears in a range of areas[10]. He is most well-known for his discovery of the T^4 radiation law. It was widely known that radiation was not proportional to the temperature difference, especially at high temperatures. Although various models were proposed, and some were widely incorporated, Stefan felt that they were not particularly good. So he compiled the data from a number of different experiments and postulated his T^4 model. This model was due in large part to the experiments by Tyndall, who performed experiments on heated platinum wire. There were flaws in Tyndall's data, which by happy circumstance cancelled out, allowing Stefan to postulate the correct dependence of the energy on the temperature for this mode of heat transfer. Boltzmann subsequently derived the relation from thermodynamic principles, and the T^4 law is known as the Stefan-Boltzmann law[11].

As a member of the Austrian Academy of Sciences, Stefan was privy to the latest scientific data. At one meeting, he heard a talk given by Karl Weyprecht, a leader of the Austro-Hungarian Polar Expedition, who presented data on the rate of ice growth in the Polar Sea. Based on this information, as well as the data presented by similar expeditions, Stefan became interested in modeling solid-liquid phase change. The difficulties of this problem lay in the time dependent, moving boundaries, which locations were not known *a priori*. By performing an energy balance across the interface between the solid and liquid phases, Stefan was able to model the growth rate of the solid[12]. This moving boundary problem is now called the Stefan problem, and the associated dimensionless variable is called the Stefan number. However, Stefan was not aware that the same problem had been already independently investigated by Lamé and Clapeyron as well as Neumann. So Stefan's name lives on for work that he did not do first, or was based on flawed data.

Despite the contributions of both Stefan and Loschmidt, they are not properly recognized for the experimental data they produced to verify the kinetic theory of gases. Loschmidt's work on the diffusion of gases and Stefan's on the diffusion of heat gave Maxwell the impetus to expand and expound his kinetic theory. He wrote first, "Professor Loschmidt, of Vienna, has recently made a series of most valuable and accurate experiments on the interdiffusion of gases ... these results I consider to be the most valuable hitherto obtained as data for the construction of a molecular theory of gases."[13] He then followed, "Prof. Stefan of Vienna, has recently, by a very delicate method, succeeded in determining of

the conductivity of air, and he finds it, as he tells us, in striking agreement with the value predicted by the [kinetic] theory."[14]

Despite being in close contact for most of their productive years, these two friends and colleagues have since been recognized in vastly different ways.

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The author gratefully acknowledges the help and hospitality of Wolfgang L. Reiter.

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[3]Janez Strnad, *Jozef Stefan: The Centenary of His Death*, (Ljubljana, 1993).

[4]Alfred Bader and Leonard Parker, "Joseph Loschmidt, Physicist and Chemist", *Physics Today*, **54** (2001), pp. 45-50.

[5]Stephen M. Stigler, "Stigler's Law of Eponymy", *Science and Social Structure*, (New York: New York Academy of Sciences, 1980), pp.147-157.

[6]Josef Loschmidt, "Konstitutionformeln der Organische Chemie in Graphischer Darstellung", *Chemische Studien I.*

[7]Alfred Bader, "Loschmidt's Graphical Formulae of 1861", in *Pioneering Ideas for the Physical and Chemical Sciences: Josef Loschmidt's Contributions and Modern Development in Structural Organic Chemistry*, W. Fleischhacker and T. Schönfeld, eds. (New York and London: Plenum, 1997), pp. 65-80.

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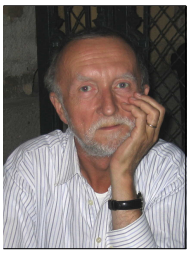
Remarks on Boltzmann's Philosophy

Wolfgang L. Reiter



Although Boltzmann's writings on the philosophy of science and epistemology belong to his lesser-known and little-discussed legacy, he made important contributions to this field, presenting a theory of scientific change that was inspired by Darwin's theory of evolution. He even speculated on an extension of physical theory to biology, recognising that there is no contradiction between biological evolution and the laws of thermodynamics.[1] For the famous 10th (1902) edition of the *Encyclopaedia Britannica* Boltzmann wrote an article on "Model", extending his earlier writings on pictures.[2]

In Defense of Atomism

Around the time when Boltzmann moved to Leipzig, both the concept and the consistency of atomism were challenged on physical as well as philosophical grounds. The reversibility and recurrence paradoxes and the problem of specific heat weakened the credibility of atomistic theories. Moreover, Boltzmann's atomism was put into question by the "energetics" doctrines represented by Ostwald and the theoretical physicist Georg Helm (1851–1923) from Dresden, with Mach in the background as their somewhat reluctant godfather regarding "energetics". The energeticists' positivistic view and phenomenological (Machian) epistemology discarding atomism had their complement in Pierre Duhem's (1861–1916) positivistic approach of thermodynamics. Furthermore, Henri Poincaré (1854–1912) was not a keen supporter of atomism. So, during the last decade of the 19th century the scientific community of continental Europe with Germany and France leading, turned away from atomism and philosophical materialism in favour of phenomenological and positivistic approaches. The support of the kinetic theory and atomism was restricted to supporters in England and the Netherlands.

At the *67. Versammlung der Gesellschaft der Deutschen Naturforscher und Ärzte* in Lübeck in September 1895 Ostwald, Helm and Boltzmann used the opportunity to bring their arguments before the German scientific community.[3] Boltzmann most successfully fought for atomism and the kinetic theory during a two-day debate with Ostwald and Helm and he inspired a younger generation of physicists, among them Max Planck (1858–1947) and Arnold Sommerfeld (1868–1951). Boltzmann, the "bullish" defender of his standpoint (so Sommerfeld in his often cited report on the fierce debate),[4] was not a philosophical doctrinist but rather flexible when he was reflecting on the construction of representations (models) or pictures ("Bilder"). In that respect, Boltzmann was critically following Heinrich Hertz (1857–1894) and his conception of pictures presented in the preface of his *Principles of Mechanics*.[5] Although we have no direct (written) evidence by Boltzmann himself it seems to be plausible to assume that he already had been acquainted with the notion of mental pictures or representations much earlier through the work of Robert von Zimmermann (1824–1898) and his textbook *Philosophische Propädeutik*.[6] Boltzmann studied philosophy with Zimmermann who became professor at the University of Vienna in 1861.

Hertz – Darwin – Mach

Boltzmann admired the work of Hertz but had a different view on the relation of the concept of reality and reality proper. Boltzmann criticised the existence of *a priori* valid laws of logic or knowledge, or explanations independent of our experience. Following Charles Darwin (1809–1882) Boltzmann's evolutionist conception of epistemology did not allow for such laws of knowledge.

> *What then will be the position of the so-called laws of thought in logic? Well, in the light of Darwin's theory they will be nothing else but inherited habits of thought.*[7]

This passage in his polemics against Schopenhauer of 1905 sounds like the programmatic statement of one of the fol-

lowers of evolutionary epistemology in the eighties of the last century. Darwin was a strong ally for his mechanistic, i.e. materialistic world view:

> *In my view all salvation for philosophy may be expected to come from Darwin's theory. As long as people believe in a special spirit that can cognize objects without mechanical means, or in a special will that likewise is apt to will that which is beneficial to us, the simplest psychological phenomena defy explanation.*
>
> *Only when one admits that spirit and will are not something over and above the body but rather the complicated action of material parts whose ability so to act becomes increasingly perfected by development, only when one admits that intuition, will and self-consciousness are merely the highest stages of development of those physicochemical forces of matter by which primeval protoplasmic bubbles were enabled to seek regions that were more and avoid those that were less favourable for them, only then does everything become clear in psychology.*[8]

For Boltzmann strong philosophical convictions, like Hertz' apriorism or Mach's phenomenology, were of little use in physics. Boltzmann in a very pragmatic way was led by the power of physical models of explanation (his "Bilder") justified by mathematical consistency. What Boltzmann probably had in mind when he was referring to pictures or models was an "isomorphism" between the structural elements of a physical proposition and the attributed mathematical elements but strongly guided (or modeled) by pictures or visualizable representations. Opposing Mach's epistemological anti-realism and empiricism Boltzmann's position was that of a realist. But his epistemological realism was not a naive realism equating physical models ("Bilder") with direct representations of reality. One even is tempted to find traits of an instrumentalism in Boltzmann's writings when he presents the atomistic hypothesis as the most convincing and comprehensive, simple and elegant description of the natural phenomena.

In his lecture on the *"Development of methods of theoretical physics"* delivered at the *71.Versammlung der Gesellschaft der Deutschen Naturforscher und Ärzte* in Munich in September 1899 Boltzmann remarks:

> *[...] namely that no theory can be objective, actually coinciding with nature, but rather that each theory is only a mental picture of phenomena, related to them as sign is to designatum. From this it follows that it cannot be our task to find an absolutely correct theory but rather a picture that is, as simple as possible and that represents phenomena as accurately as possible.*[9]

And he concluded:

> *The question whether matter consists of atoms or is continuous reduces to the much clearer one, whether [the conception of enormously many individuals or that of] the continuum is able to furnish a better picture of phenomena.*[10]

Moreover, Boltzmann's ontological position regarding atoms was flexible and he repeatedly made clear that he preferred an open and pragmatic attitude. In his discussion on the identity of psychic processes with certain material processes in the brain Boltzmann adds a most remarkable endnote:

> *That is, if the concept of continuum is properly understood, an interplay of its atoms, by which of course we must not imagine material points but perhaps vectors or whatever. Nor do the atoms necessarily have to be immutable.*[11]

Theories of the continuum had been regarded in Boltzmann's times as phenomenological theories in opposition to atomistic theories and hence atomism was not a phenomenological theory. What Boltzmann is telling us here in defence of atoms is the fact that continuum mechanics — if *"properly understood"* — also has to go beyond pure phenomenology by assuming its own "atoms", *"perhaps vectors or whatever"*. On the methodological level Boltzmann's mechanical atom is represented by a picture ("Bild") central to his mechanistic (realistic) world view. On the epistemological level he is cautious enough not to identify his mechanical atoms with the real world out there.

> *Über die Beschaffenheit der Atome aber wissen wir noch gar nichts und werden auch solange nichts wissen, bis es uns gelingt, aus den durch die Sinne beobachtbaren Tatsachen eine Hypothese zu formen.* [12]

And he prophetically remarks in this essay of 1886:

> *Merkwürdigerweise ist hier am ersten wieder von der Kunst Erfolg zu hoffen, welche sich auch bei Erforschung der Himmelskörper so mächtig erwies, von der Spektralanalyse.*[13]

New Physics

His farsighted consideration of spectral analysis as a powerful tool to reveal the inner structure of atoms, *"...die Beschaffenheit der Atome..."*, of 1886 is in sharp contrast to the observation that he never mentioned the phenomena of radioactivity discovered twelve years later. This is puzzling because as a member of the Vienna Academy of Sciences he was well informed about the seminal role Vienna played in fostering radioactivity research in Paris in supplying the Curies in 1898–99 with more then one ton of pitchblend residues from the then Austrian uranium mine in St. Joachimsthal (now Jachimov, Czech Republic), which enabled Marie Curie (1867–1934) and Pierre Curie (1859–1906) to discover polonium and radium. Moreover, with their work in 1899, Stefan Meyer (1872–1949) and Egon von Schweidler (1873–1948), both Boltzmann's students at the Vienna institute, correctly distinguished between the radiation from radium (α-rays) and from polonium (β-rays) by their different behaviour in a magnetic field. (The electromagnet had been available at Boltzmann's institute.) They proved that the deflection of the radium rays was identical to that of cathode rays, that is, that the radium rays consist of negatively charged particles. This led to the fundamental insight of the corpuscular nature of these rays which is strong experimental support of the atomistic nature of these new phenomena.[14] Although Boltzmann wrote a popular account on X–rays

a few month after their discovery by Konrad Röntgen (1854–1923),[15] he never mentioned the ongoing work on radioactivity research at his own institute. Probably he took notice of the recent developments and just did not comment on them, but it seems more likely that he had lost interest in actual physical research during his last years. In his *Lectures on Natural Philosophy* 1903 – 1906 he did not present anything referring to new physics. During the last decade of his life he no longer contributed to the forefront of research but commented on what he had achieved and tried to secure his work in writing monographs and popular articles.

Throughout his life Boltzmann was very interested in technology. He considered technological progress as a confirmation of the sciences.

> *That is why I do not regard technological achievements as unimportant by-products of natural science but as a logical proof. Had we not attained these practical achievements, we should not know how to infer. Only those inferences are correct that lead to practical success.*[16]

In fact Boltzmann argues here as a scientific realist (and atomist) implicitly against idealism (and phenomenological anti-atomism) in taking the progress of science (and technology) as a confirmation of his epistemological position – realism. So, the growing experience and the accumulation of increasingly refined knowledge produced by science (and applied by technology) corroborate realism. Despite of Boltzmann's strong anti-metaphysical sentiments his own concept of realism is part of a metaphysical concept. Probably, Boltzmann was quite aware of that fact and therefore disguised his epistemological realism as a methodological principle, in sharp contrast to Mach's concept. What I mean by disguising realism is Boltzmann's view of the conception of pictures ("Bilder") as representations of the "world out there". Admittedly, since Boltzmann never has developed his philosophy of science in a systematic manner, his ideas are a profound source of various interpretations and misunderstandings.

What makes reading his *Populäre Schriften* such a delightful experience is Boltzmann's humour. In a slightly poetic manner Boltzmann speaks about the power of theory.

> *The gigantic structures of the Brooklyn Bridge that stretches beyond sight and the Eiffel tower that soars without end rest not only on the solid framework of wrought iron, but on the solider one of elasticity theory.*[17]

In 1894, at the *66. Versammlung der Gesellschaft der Deutschen Naturforscher und Ärzte* in Vienna he gave a lecture "On Airship Flight" (*"Über Luftschiffahrt"*), on flying objects heavier than air by demonstrating models of aeroplanes of the Austrian aeronautics pioneer Wilhelm Kress (1836–1913) which Boltzmann let fly around in the congregation hall of the assembly at the Vienna Musikverein.[18] Boltzmann was correct in his clear-sighted prediction that not airships but aeroplanes would be the superior technology of the future.

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[4] *"Das Referat für die Energetik hatte Helm - Dresden; hinter ihm stand Wilhelm Ostwald, hinter beiden die Naturphilosophie des nicht anwesenden Ernst Mach. Der Opponent war Boltzmann, sekundiert von Felix Klein. Der Kampf zwischen Boltzmann und Ostwald glich, äusserlich und innerlich, dem Kampf des Stieres mit dem geschmeidigen Fechter. Aber der Stier besiegte diesmal den Torero trotz all seiner Fechtkunst. Die Argumente Boltzmann's schlugen durch. Wir damals jüngeren Mathematiker standen auf der Seite Boltzmann's; es war uns ohne weiters einleuchtend, dass aus der einen Energiegleichung unmöglich die Bewegungsgleichungen auch nur eines Massenpunktes, geschweige denn eines Systems von beliebigen Freiheitsgraden gefolgert werden könnten."*Arnold Sommerfeld, *Das Werk Boltzmann's*. Lecture at the occasion of Ludwig Boltzmann's 100th birthday. Quoted in Erhard Scheibe, *Die Philosophie der Physiker.* (ref. 33), pp.105-106.

[5]Heinrich Hertz, *Die Prinzipien der Mechanik in neuem Zusammenhange dargestellt.* Gesammelte Werke, Band III. (Leipzig: Johann Ambrosius Barth, 1894), pp. 1-5; reprinted in Ostwalds Klassiker Vol. 263. (Frankfurt am Main: Verlag Harri Deutsch, 2. Auflage 1996.)

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[8]ibid., in *Populäre Schriften.* (ref. 10), pp. 385-402; eingeleitet und ausgewählt von Engelbert Broda (ref. 36), pp. 240-257, on page 251; translated into English in Brian McGuinness (ed.), (ref. 36), pp. 185-198, on page 193.

[9] *"[...] dass keine Theorie etwas Objektives, mit der Natur wirklich sich Deckendes sein kann, dass vielmehr jede nur ein geistiges Bild der Erscheinung ist, das sich zu diesem verhält, wie das Zeichen zum Bezeichneten. Daraus folgt, dass es nicht unsere Aufgabe sein kann, eine absolut richtige Theorie, sondern vielmehr ein möglichst einfaches, die Erscheinungen möglichst gut darstellendes Abbild zu finden."* Ludwig Boltzmann, "Über die Entwicklung der Methoden der theoretischen Physik in neuerer Zeit". in *Populäre Schriften.* (ref. 10), pp. 198-277; eingeleitet und ausgewählt von Engelbert Broda (ref. 36), pp. 120-149, on page 137; translated into English in Brian McGuinness (ed.), (ref. 36), pp. 77-100, on page 90.

[10] *"Die Frage, ob die Materie atomistisch zusammengesetzt oder ein Kontinuum ist, reduziert sich auf die viel klarere, ob die Vorstellung enorm vieler Einzelwesen oder die eines Kontinuums ein besseres Bild der Erscheinungen zu liefern vermöge."* Ludwig Boltzmann, "Über die Entwicklung der Methoden der theoretischen Physik in neuerer Zeit". in *Populäre Schriften.* (ref. 10), pp. 198-277; eingeleitet und ausgewählt von Engelbert Broda (ref. 36), pp. 120-149, on page 138; translated into English in Brian McGuinness (ed.), (ref. 36), pp. 77-100, on page 91.Insertion in brackets [...] is added by the author.

[11] *"D. h. bei richtiger Auffassung des Begriffs des Kontinuums ein Spiel der Atome desselben, worunter man sich freilich nicht materielle Punkte denken muss, sondern vielleicht Vektoren oder wer weiss was. Auch müssen die Atome nicht notwendig unveränderlich sein."* Ludwig Boltzmann, "Über die Frage nach der objektiven Existenz der Vorgänge in der unbelebten Natur". in *Populäre Schriften.* (ref. 10), pp. 162-187; eingeleitet und ausgewählt von Engelbert Broda (ref. 36), pp. 94-119, on page 112; translated into English in Brian McGuinness (ed.), (ref. 36), pp. 57-76, on page 76.

[12]Ludwig Boltzmann, "Der zweite Hauptsatz der mechanischen Wärmetheorie". in *Populäre Schriften*. (ref. 10), pp. 25-50, on p. 30; eingeleitet und ausgewählt von Engelbert Broda (ref. 36), pp. 26-46, on page 31; translated into English in Brian McGuinness (ed.), (ref. 36), pp. 5713-32, on page 17; here the translation is highly misleading.

[13]Ibid., the passage cited here in German is missing in the English translation.

[14]St. Meyer and E. v. Schweidler, "Über das Verhalten von Radium und Polonium im magnetischen Felde," Anzeiger der kaiserl. Akad. d. Wiss., mathem.- naturw. Kl. 22 (November 3, 1899), 1-4.

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[15]Ludwig Boltzmann, "Röntgens neue Strahlen" in *Populäre Schriften*. (ref. 10), pp. 188-197.

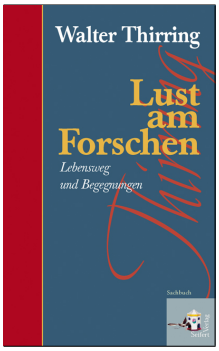
[16]*"Deshalb halte ich die Errungenschaften der Technik nicht für nebensächliche Abfälle der Naturwissenschaften, ich halte sie für logische Beweise. Hätten wir diese praktischen Errungenschaften nicht erzielt, so wüssten wir nicht, wie man schliessen muss. Nur solche Schlüsse, welche praktischen Erfolg haben, sind richtig"*. Ludwig Boltzmann, "Eine These Schopenhauers". in *Populäre Schriften.* (ref. 10), pp. 385-402; eingeleitet und ausgewählt von Engelbert Broda (ref. 36), pp. 240-257, on page 249; translated into English in Brian McGuinness (ed.), (ref. 36), pp. 185-198, on page 193.

[17]*Der Riesenbau der Brooklyner Brücke, welche sich unabsehbar in die Länge, und der des Eifelturms, der sich endlos in die Höhe erstreckt, sie beruhen nicht bloss auf dem festen Gefüge des Schmiedeeisens, sondern auf dem festeren der Elastizitätstheorie.*Ludwig Boltzmann, "Über die Bedeutung von Theorien". in *Populäre Schriften.* (ref. 10), pp. 76-80; eingeleitet und ausgewählt von Engelbert Broda (ref. 36), pp. 54-58, on page 56; translated into English in Brian McGuinness (ed.), (ref. 36), pp. 33-36, on page 35.

[18]Ludwig Boltzmann, "Über Luftschiffahrt", in *Populäre Schriften*, (ref. 10), pp. 81-91. As a mere curiosity I note, that Ludwig Wittgenstein (1889–1951) who considered Boltzmann's philosophical writings as an important influence on his own thinking first studied mechanical engineering at the Technische Hochschule in Charlottenburg, Berlin for two years before he went to Manchester where he studied aeronautics.

ESI News

Walter Thirring: ***Autobiography***



Walter Thirring, founding father and Honorary President of the ESI, has written an autobiography. The book is on the market in December this year.

Walter Thirring, Lust am Forschen – Lebensweg und Begegnungen. Wien: Seifert Verlag 2008.

New Members of the ESI Society 2008:

Markus Arndt (Faculty of Physics, University of Vienna)
Reinhard Bürger (Faculty of Mathematics, University of Vienna)
Joachim Hermisson (Faculty of Mathematics, University of Vienna)

New activity in history and philosophy of science:

Jaques Bouveresse (College de France)

gave a lecture on *"Ludwig Boltzmann und das Problem der Erklärung in der Wissenschaft"* on Oktober 29, 2008 at the Boltzmann Lecture Hall of the ESI. This lecture was preceded by a lecture on *"Musil als Philosoph"* at the Kleiner Festsaal at the main building of the University of Vienna. The lecture was organized in cooperation with the Institute for Philosophy, University of Vienna, and the Institute Vienna Circle by E. Nemeth, W. L. Reiter and F. Stadler.

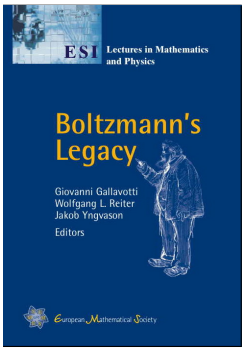
International Workshop "Routes to Mauthausen", November 27 to November 29, 2008.

The Workshop was organized by Gerhard Botz (Professor for Contemporary History, Faculty for Historical and Cultural Studies, University of Vienna and Ludwig Boltzmann Institute for Historical Social Science). The workshop was opened by a Round Table Discussion on *"Humanity and the Experience of Violence and Genocide"* on November 27, 2008 at the premisses of the ESI.

New ESI Lectures in Mathematics and Physics

Boltzmann's Legacy

G. Gallavotti, W. L. Reiter, J. Yngvason (eds.)
Zürich: European Mathematical Society Publishing House 2008.



This book contains lectures presented at the International Symposium *"Boltzmanns Legacy"* held at the ESI in June 2006 to commemorate the 100th anniversary of Ludwig Boltzmann's death in Duino.
The text covers a broad spectrum of topics ranging from equilibrium and nonequilibrium statistical physics, ergodic theory and chaos to basic questions of biology and historical accounts of Boltzmann's work. Besides the lectures presented at the symposium the volume also contains contributions specially written for this occasion. The articles give a broad overview of Boltzmann's legacy to the sciences from the standpoint of some of present day's leading scholars in the field.

The book addresses students and researchers in mathematics, physics and the history of science.

News from the Scientific Community

Markus Arndt

(Speaker of the group Quantum Optics, Quantum Physics and Quantum Information of the Faculty of Physics, University of Vienna), member of the ESI society, was awarded the **Wittgenstein Price 2008**.

Arndt already has won the START-Price of the FWF 2001.

Markus Aspelmeyer (Institut for Quantum Optics and Quantum Information - IQOQI, ÖAW Vienna), **Massimo Fornasier** (Johann Radon Institute for Computational and Applied Mathematics, ÖAW Linz) and **Daniel Grumiller** (Institut für Theoretische Physik, Vienna University of Technology) had been awarded the **Start Price** of the FWF 2008.

All friends of the ESI are cordially invited to a Christmas Party at the Institute on Thursday, December 18, 2008, 5.00 p.m.

Current and Future Activities of the ESI

Thematic Programmes 2008

Combinatorics and Statistical Physics, February 1 – June 15, 2008

Organisers: M. Bousquet-Melou, M. Drmota, C. Krattenthaler, B. Nienhuis

Workshop, May 25 – June 7, 2008

Summer School, July 7 – July 18, 2008

Metastability and Rare Events in Complex Systems, February 1 – April 30, 2008

Organizers: P.G. Bolhuis, C. Dellago, E. van den Eijnden

Workshop, February 17 – February 23, 2008

Hyberbolic Dynamical Systems, May 12 – July 5, 2008

Organisers: H. Posch, D. Szasz, L.-S. Young

Workshop, June 15 – June 29, 2008

Operator Algebras and Conformal Field Theory, August 25 – December 15, 2008

Organisers: Y. Kawahigashi, R. Longo, K.-H. Rehren, J. Yngvason

Thematic Programmes 2009

Representation theory of reductive groups — local and global aspects, January 2 – February 28, 2009

Organizers: G. Henniart, G. Muic and J. Schwermer

Mathematics at the Turn of the 20th Century: Explorations and Beyond, January 7 - 12, 2009

Organizers: D.D Fenster, J. Schwermer

Number theory and physics, March 1 - April 18, 2009

Organizers: A. Carey, H. Grosse, D. Kreimer, S. Paycha, S. Rosenberg and N. Yui

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Gravity in Three Dimensions, April 14 - 24, 2009

Organizers: H. Grosse, D. Grumiller, R. Jackiw, D. Vassilevich

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Selected topics in spectral theory, May 4 – July 25, 2009

Organizers: B. Helffer, T. Hoffmann-Ostenhof and A. Laptev

Catalysis from First Principles, May 25 - 30, 2009

Organizers: J. Hafner, J. Norskov, M. Scheffler

Large cardinals and descriptive set theory, 2 weeks in June – July 2009

Organizers: S. Friedman, M. Goldstern, R. Jensen, A. Kechris and W.H. Woodin

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Entanglement and correlations in many-body quantum mechanics, August 18 – October 17, 2009

Organizers: B. Nachtergaele, F. Verstraete and R. Werner

The dbar-Neumann problem: analysis, geometry and potential theory, October 27 - December 24, 2009

Organizers: F. Haslinger, B. Lamel, E. Straube

Thematic Programmes 2010

Quantitative Studies of Nonlinear Wave Phenomena, January 7 - February 28, 2010

Organizers: P.C. Aichelburg, P. Bizon, W. Schlag

Quantum field theory on curved space-times and curved target-spaces, March 1 - April 30, 2010

Organizers: M. Gaberdiel, S. Hollands, V. Schomerus, J. Yngvason

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Matter and radiation, May 3 - July 30, 2010

Organizers: V. Bach, J. Frhlich, J. Yngvason

Topological String Theory, Modularity and Non-Perturbative Physics, June 7 - August 15, 2010

Organizers: L. Katzarkov, A. Klemm, M. Kreuzer, D. Zagier

Anti - de Sitter holography and the quark-gluon plasma: analytical and numerical aspects, August 2 - October 29, 2010

Organizers: A. Rebhan, K. Landsteiner, S. Husa

Higher Structures in Mathematics and Physics, August 15 - November 15, 2010

Organizers: A. Alekseev, H. Bursztyn, T. Strobl

Other Scientific Activities in 2008

Tensor network methods and entanglement in quantum many-body systems, January 16 – January 18, 2008

Organizers: F. Verstraete, G. Vidal and M. Wolf

Ab-initio density-functional studies of intermetallic compounds, January 23 – January 25, 2008

Organizer: J. Hafner

15th Anniversary of the ESI, April 14, 2008

Organizers: W.L. Reiter, K. Schmidt, J. Schwermer and J. Yngvason

Frontiers in Mathematical Biology: Mathematical population genetics, April 14 – April 18, 2008

Organizers: R. Bürger and J. Hermisson

Topics in Mathematical Physics, July 21 – July 31, 2008

Organizers: C. Hainzl, R. Seiringer and J. Yngvason

Vienna Central European Seminar on Particle Physics and Quantum Field Theory, November 28 – November 30, 2008.

The topic of the Seminar is **"Highlights in Computational Quantum Field Theory"** and is opened by a public lecture on **"Quarks, Gluons, and Lattices"** by Michael Creutz, BNL, on November 28, 2008.

This Semininar, organized by the Faculty of Physics, University of Vienna, is supported by the ESI.

Organizer: H. Hüffel

Supersymmetry and Noncommutative Quantum Field Theory. In memoriam Julius Wess, December 4 - 6, 2008.

Organizers: H. Grosse, P. Schupp

Profinite Groups, December 7 – December 20, 2008

Organizers: K. Auinger, F. Grunewald, W. Herfort and P.A. Zalesski

Erwin Schrödinger Lectures

Autumn Term 2008/09

The Erwin Schrödinger Lectures are directed towards a general audience of mathematicians and physicists. In particular it is an intention of these lectures to inform non-specialists and graduate students about recent developments and results in some area of mathematics or mathematical physics.

These lectures take place in the Boltzmann Lecture Room of the ESI.

Each lecture will be followed by an informal reception at the Common Room of the ESI.

Vaughan Jones (UC Berkeley): *Flatland, a great pleasure to do algebra.* Nov 4, 2008

Matthias Kreck (Hausdorff Research Institute, Bonn): *Codes and 3-dimensional manifolds.* Nov 13, 2008

Jean-Pierre Serre (College de France, Paris): *Variation with p of the number of solutions (mod p) of polynomial equations.* Dec 11, 2008

James W. Cogdell (Ohio State University, Columbus): *On sums of three squares.* Jan 22, 2009

Organizer: J. Schwermer

Senior Research Fellows Lecture Courses

Autumn and Spring Term 2008/09

To stimulate the interaction with the local scientific community, the ESI offers lecture courses on an advanced graduate level. These courses are taught by Senior Fellows of the ESI, whose stays in Vienna are financed by the University of Vienna, the Vienna University of Technology, and the Austrian Federal Ministery for Education, Science and Culture.
These courses take place in the Erwin-Schrödinger Lecture Room of the ESI.

Goran Muic (University of Zagreb): *Selected Topics in the Theory of Automorphic Forms for Reductive Groups* Thursday, 13:00-15:00, starting on October 16, 2008

Feng Xu (University of California, Riverside): *Operator Algebras and Conformal Field Theory* Wednesday and Friday, 16:00-18:00, starting on November 4, 2008

Nigel Higson (Penn State University): *Index Theory, Groupoids and Noncommutative Geometry* Monday and Wednesday, 14:00-16:00, Friday 10:30-12:30, starting on November 24, 2008

Michel Loss (Georgia Tech): *Inequalities* April 15 - June 30, 2009

Raimar Wulkenhaar (Münster): *Spektraltripel in der nichtkommutativen Geometrie und Quantenfeldtheorie* March 1 - June 15, 2009

Mathematics at the Turn of the 20th Century: Explorations and Beyond

January 7 - 12, 2009

This workshop aims to bring together scholars from a variety of fields with a common interest in the mathematical sciences of the 19th and 20th centuries in their historical context. Special attention will be given to include young participants. The programme will combine lectures on recent results with ample time for informal discussions and collaborations. In commemoration of Hermann Minkowski's death on January 12, 1909, the talks given on Monday, January 12, 2009 will illuminate Minkowski's work in mathematics and physics.

Among these talks are:

Scott Walter (Nancy): *Hermann Minkowski and theoretical physics in Göttingen*

Samuel J. Patterson (Göttingen): *The number-theorist Hermann Minkowski*

Organizers: D. D Fenster, J. Schwermer

Editors: Wolfgang L. Reiter, Klaus Schmidt, Joachim Schwermer, Jakob Yngvason

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