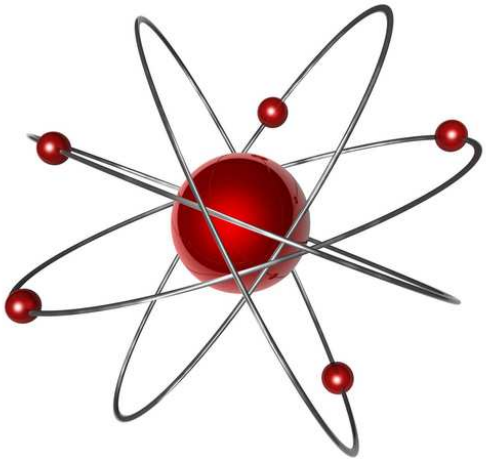
International Association of Mathematical Physics

News Bulletin

January 2012



International Association of Mathematical Physics News Bulletin, January 2012

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Cover photo: The Rutherford-Bohr model of the atom made an *analogy* between the Atom and the Solar System. (The artistic picture is "Solar system" by Antar Dayal.)

Tasks ahead

by Antti Kupiainen (IAMP President)

The elections for the Executive Committee of the IAMP for the coming three years were held last fall and the new EC started its work beginning of this year. I would like to thank on behalf of all of us in the EC the members of IAMP for choosing us to steer our Association during the coming three years.

I would also like to thank the previous EC for its work to the benefit of our community. In particular there are two reforms they carried out that the new EC should continue with. The first one concerns the the IAMP News Bulletin that has become an interesting "official" journal for our community. We should certainly give all our support to the editorial board so that they can continue the good work they have done so far.

As a consequence of the membership reform we have now over 640 paying members which means that our finances are on a reasonably solid ground. However our age distribution is still too heavily tailed, and we should actively recruit younger researchers. The IAMP was originally founded in 1976 to promote the interests of the new mathematical physics community. The community had grown strongly after the late 60's and had a strong sense of mission and common interests. Many were doing research genuinely combining mathematics and physics and found it hard to define themselves to be only physicists or only mathematicians, which was assumed if applying for a job in a physics or a mathematics department. Since those days the community has grown much more heterogenous. There are more people with a pure mathematics background but excited about problems coming from physics or physicists needing cutting edge mathematics. There is no reason IAMP couldn't attract such people and we should do all we can to have more of them join our community. There are also simple things that require very little effort each of us can do. Tell your collaborators, visitors etc. about IAMP. Encourage your students and postdocs to join.

A major factor that helps to build cohesion in our community is of course our congress held every three years and taking place this year in Aalborg, Denmark. I hope as many of our members as possible will participate. In particular I urge you to send your PhD students to the meeting and to the Young Researcher Symposium immediately preceding the meeting.

Although the 2012 congress is still ahead of us it is already time to think about the 2015 meeting as well whose site will be chosen in the General Assembly in Aalborg. I would encourage everybody who thinks they are in a position to be able to make a bid seriously consider this. Out of the 16 ICMP's organized so far only 4 have not been in Europe. This distribution is not an accurate representation of the geographic origin of our members. Therefore bids to organize ICMP 2015 outside of Europe would be particularly welcome!

A centennial of Rutherford's Atom

by Rafael D. Benguria (Santiago de Chile)

Rafael Benguria got his Ph.D. in Physics from Princeton University in 1979. He is a Professor at the Physics Department of P. Universidad Católica de Chile. He has done research in Schrödinger Operators, Spectral Geometry, Stability of Matter Problems, and Nonlinear PDE's. Rafael Benguria has belonged to the IAMP since 1979 and was part of its Executive Committee from 2006–2011.

On March 22, 2011, the New York Times published the article *"A Nucleated Century"* on its Editorial page, celebrating the hundredth anniversary of Rutherford's 1911 manuscript [23]. The quoted article read at the start: "*...If you asked someone to draw an atom, he or she would probably draw something like a cockeyed solar system (see Figure 1). The sun – the nucleus – is at the center, and the planets – the electrons – orbit in several different planes. The critical discovery in this atomic model emerged a century ago in a talk before the Manchester Literary and Philosophical Society in March 1911 and a paper published soon after in the Philosophical Magazine. Both were by Ernest Rutherford, who had won the 1908 Nobel Prize in Chemistry in part for his discovery of the alpha particle, which he later proved was the nucleus of a helium atom...*". The title of New York Times editorial article emphasized the discovery of the nucleus of the atom, and the beginnings of Nuclear Physics, which is certainly a true fact. On the other hand, the 1911 article of Rutherford did much more than that: it gave rise to modern atomic physics and it contributed enormously to push the beginnings of Quantum Mechanics.

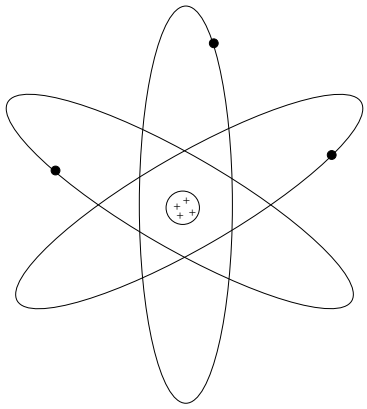

Figure 1

Although conceived more like a philosophical idea by Democritus of Abdera and others in Ancient Greece, the idea that matter is formed by atoms was first used in Physics by Daniel Bernoulli at the beginning of the XVIIIth century to obtain from first

principles in microscopic physics the law of ideal gases, giving birth to Kinetic Theory (later developed to full extent by Maxwell and Boltzmann in the XIXth century). The discovery of photosynthesis by Jan Ingenhousz and Joseph Priestley in 1779 [16] prompted the discovery of oxygen, the introduction of the idea of chemical elements by Lavoisier, and the foundations of *modern chemistry* by John Dalton [8]. By that time, the concept of atoms was taking a proper place in physics and chemistry, and these atoms were much more than just small bodies whose restless motion would explain thermodynamic quantities like temperature and pressure. They had a structure, they could combine to form molecules, and the rules for combination were laid down by Dalton.

During the XIXth century there were contributions from many people in different disciplines of physics that shed some light on the rich structure of the atom. In March of 1820 a crucial experiment of Hans Christian Oersted showed that Electricity and Magnetism were not independent phenomena [19], and that one could produce a magnetic field by driving a current through an electric circuit. Electromagnetism was born, and with it an extraordinary chain of pure and applied discoveries, including the first electric motors, which culminated in August of 1831, with the discovery of electromagnetic induction by Michael Faraday. A key figure of this period was Ampère who, among many contributions, introduced the idea of microscopic currents inside a metal to make the connection between Oersted's experiment and the properties of a magnet. The discovery of electrolysis by Humphry Davy, and the crucial observation by Michael Faraday that the amount of matter deposited on the cathodes of the electrolysis experiment is proportional to the total charge (current times time) applied to the electric terminals was the first experimental observation that electric charge in matter is quantized. In the meantime many key ideas were crystalizing in chemistry, among them, the introduction of the Avogadro number in 1811 [1] (i.e., when gaseous masses, at the same temperature and pressure, occupy equal volumes, they all contain the same number of molecules), the observation of Proust that the mass of any chemical element is an integer number times the mass of hydrogen, and the skilled accumulated work by many people on chemical reactions that lead D. Mendeleev to establish the Periodic Table of Chemical Elements in 1869.

It was clear from all the previous observations that atoms and molecules ought to have an internal structure, yet to be discovered, that could explain these experimental facts. Still a whole new set of experiments and ideas would enter into the picture and help understanding this internal structure. These came from studying the interaction of light with matter. Using the idea of Newton that light could be decomposed into different colors by letting it pass through a prism, Wollaston and Fraunhofer introduced the field of spectroscopy, and determined the typical emission lines of incandescent gases. Moreover, in 1859, Gustav Kirchhoff posed the problem of determining the spectral decomposition of light emitted by a heated body. Then, in 1887, Heinrich Hertz [15] discovered the photoelectric effect, i.e., the emission of an electric spark by a metal plate when illuminated by visible or ultraviolet light. The intensity of this spark was larger, the higher the frequency of the incident light.

During the last decade of the XIXth century and the first one of the XXth century, the study of these three problems gave birth to the new Quantum Physics. In 1885, J. Balmer [2] classified the spectrum of Hydrogen in a simple phenomenological expression, which started to put some order in the huge experimental literature in atomic spectroscopy. By 1896, W. Wien, gave the first answer for the black body radiation [27], which reproduced appropriately the experimental data available at the time. However, better experimental results due to Kurlbaum, Pringsheim, and Rubens in 1900, showed small disagreements, at low frequencies, with Wien's theoretical results. In fact, for low frequencies, the experimental results were in agreement with the recent results of Jeans and Rayleigh (based on the spectral asymptotics of the eigenfrequencies of electromagnetic cavities). By October of 1900, M. Planck [22] derived an interpolation between Wien's results (for high frequency) and the Rayleigh–Jeans results (for low frequency), which reproduced very precisely the experimental curves of Kurlbaum, Pringsheim, and Rubens. Planck's formula for the emission of a black body marked the beginning of Quantum Physics. In 1905, Albert Einstein [11], introduced the quanta of light (i.e., the present day *photons*) to explain the experimental results of H. Hertz on the photoelectric effect. The same year Einstein [12] gave a solution to the Brownian motion problem (observed independently by Robert Brown in 1827, and by Jan Ingenhousz in 1784), showing that the root mean square displacement of a Brownian particle is proportional to time, and that the diffusion constant is inversely proportional to the Avogadro Number. This dependence of the diffusion constant allowed Perrin [20] to make the first accurate experimental determination of the Avogadro number (see also [21], and the review article of Duplantier [10]).

In the meantime, the discovery of radioactivity by H. Becquerel in 1896 [3] and the electron by J. J. Thomson in 1897 [25], prompted a renewed interest in trying to determine the internal structure of atoms. Thus, at the beginning of the XXth century several people (including J .J. Thomson [26], and H. Nagaoka [18]), introduced different models of atoms (basically neutral systems with positive and negative charge distributions interacting via a Coulomb potential). It is at this point in this history that Rutherford's contributions enters. By 1907, Ernest Rutherford had become a successor of Arthur Schuster (a leading spectroscopist of the time) as Professor of Physics at the University of Manchester. At Manchester, Rutherford continued his research on the properties of the radium emanation and of the alpha rays and, in conjunction with Hans Geiger, a method of detecting a single alpha particle and counting the number emitted from radium was devised (see the biography of Rutherford at the end of this manuscript). In order to try to determine the inner structure of the atom, Rutherford suggested to Geiger an experiment involving the scattering of alpha particles by a thin gold foil.

Collisions have always played a major role in physics. Already in 1668, The Royal Society of London established a competition in order to determine the laws of collisions in classical mechanics. The Royal Society received the memoirs of John Wallis (November 26, 1668), Christopher Wren (December 17, 1668), and Christiaan Huygens (January 4, 1668) who solved different aspects of the problem (see, e.g. [9], Chapter V). And the consideration of elastic collisions in special relativity yields the classical formula $p = mv/\sqrt{1-(v/c)^2}$, for the momentum of a relativistic particle. Even today, smashing

elementary particles at very high energy is the method to discover the physics at very small scales.

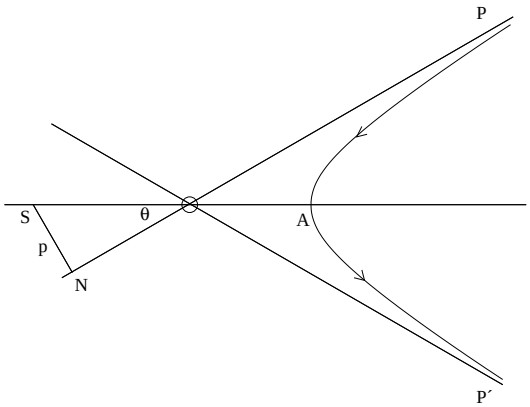

Figure 2

The gold foil experiment was conducted under the supervision of Rutherford at the University of Manchester in 1909 by Hans Geiger and the undergraduate student Ernest Marsden. In this experiment, most of the alpha particles passed straight through the foil. However, Geiger and Marsden [14] found that some alpha rays were scattered directly backwards, even from a thin film of gold. It was, a surprised Rutherford stated, "*as if one had fired a large naval shell at a piece of tissue paper and it had bounced back*". In his famous 1911 paper, Rutherford [23] starts comparing the results of the gold foil experiment with the theoretical predictions based on the Thomson model (which is usually referred to as the "plum–pudding model"), ruling it out. He then proceeds introducing the now classical picture (*the Rutherford atom*) in these words: "*...Consider an atom which contains a charge* $\pm Ne$ *at its centre surrounded by a sphere of electrification containing a charge* $\mp Ne$ *supposed uniformly distributed throughout a sphere of radius R. Here, e is the fundamental unit of charge, which in this paper is taken as* 4.65×10^{-10} *E.S. unit. We shall suppose that for distances less than* 10^{-12} *cm, the central charge and also the charge on the alpha particle may be supposed to be concentrated at a point. It will be shown that the main deductions from the theory are independent of whether the central charge is supposed to be positive or negative. For convenience, the sign will be assumed to be positive.* **The question of the stability of the atom** *proposed need not be considered at this stage, for this will obviously depend upon the minute structure of the atom, and on the motion of the constituent charged parts...*" (see [23] for details). He then calculated the scattering cross section of a charged particle by a fixed target made of a charged point (finding a dependence like $\csc(\theta/2)^4$, where θ is the deflection angle in Figure 2). Of course, Rutherford used Classical Mechanics for his computation of the scattering cross section, and he found an excellent agreement with the experimental data of the paper of Geiger and Marsden. It is a major coincidence that for the Coulomb potential, the results derived using Classical Mechanics (see, e.g., [17], p. 53, for the classical derivation), and the results using Quantum Mechanics (see, e.g., [13], Problem 110, pp. 290 ff) for the

derivation using Quantum Mechanics) are the same. This is connected with the hidden symmetry ($SO(4)$ symmetry) of the motion of a particle moving in the presence of the Coulomb field. If this were not the case, it would have been an extra (maybe impossible) puzzle to interpret the experimental results of Geiger and Marsden.

In 1911, Niels Bohr had obtained his Ph.D. at the University of Copenhagen, and joined the group of Ernest Rutherford in Manchester in 1912, attracted by the 1911 paper of Rutherford. As pointed out by Rutherford himself, his model has obvious stability problems, since in classical mechanics the accelerated electrons around the nucleus must radiate energy and fall into it in a very short time. It was in part to solve these stability problems that Niels Bohr introduced his model of the atom [4, 5, 6, 7], giving birth to the *Old Quantum Mechanics*. The *Bohr Atom* not only was an attempt to solve the stability problems of *Rutherford's Atom*, moreover, it was able to explain the Balmer series. The fact that the *semiclassical analysis* of Bohr could explain precisely the Balmer Series, and thus the spectrum of the Hydrogen Atom is again a happy coincidence due to the $SO(4)$ symmetry alluded to above.

In the century that has passed since the introduction of Rutherford's Atom [23, 24], there has been a fruitful interaction between mathematics and physics. Even in the days of the *Old Quantum Mechanics*, there were several mathematical developments carried by A. Sommerfeld and others, and with the introduction of the Schrödinger equation in 1926, the developments in Functional Analysis were growing hand by hand with Physics to help understanding the spectral properties of Atoms, Molecules and Solids. Also, in the last half a century, there has been a vast mathematical physics literature around stability problems in Atomic Physics. In summary, the introduction of the Rutherford Atom, not only marked the beginning of Nuclear Physics as stated in the *New York Times* Editorial. It also played a crucial role in Atomic Physics, and established a fertile ground for many problems in Mathematical Physics.

Ernest Rutherford was born on August 30, 1871, in Nelson, New Zealand. He received his early education in Government schools and at the age of 16 entered Nelson Collegiate School. In 1889 he was awarded a University scholarship and he proceeded to the University of New Zealand, Wellington, where he entered Canterbury College. He graduated in 1893 with a double first in Mathematics and Physical Science and he continued with research work at the College for a short time, receiving the B.Sc. degree the following year. Growing up, he often helped out on the family farm, but he was a good student. After college he won a scholarship in 1894 to become a research student at Cambridge. Upon receiving the news of this scholarship, Rutherford is reported to have said, "That is the last potato I will ever dig". At Cambridge, the young Rutherford worked in the Cavendish laboratory with J. J. Thomson, discoverer of the electron. Rutherford's talent was quickly recognized, and in 1898 he took a professorship at McGill University in Montreal. There, he identified alpha and beta radiation as two separate types of radiation, and studied some of their properties. In 1901 Rutherford and chemist Frederick Soddy found that one radioactive element can decay into another. The discovery earned Rutherford the 1908 Nobel Prize in Chemistry. Rutherford returned to England in 1907 to become Professor of Physics in the University of Manchester, succeeding Arthur Schuster, and in 1919 he accepted an invitation to succeed J. J. Thomson as Cavendish Professor of

Physics at Cambridge. At Manchester, Rutherford continued his research on the properties of the radium emanation and of the alpha rays and, in conjunction with H. Geiger, a method of detecting a single alpha particle and counting the number emitted from radium was devised. In 1910, his investigations into the scattering of alpha rays and the nature of the inner structure of the atom which caused such scattering led to the postulation of his concept of the ***nucleus***, his greatest contribution to physics. According to him practically the whole mass of the atom and at the same time all positive charge of the atom is concentrated in a minute space at the centre. In 1912 Niels Bohr joined him at Manchester and he adapted Rutherford's nuclear structure to Max Planck's quantum theory and so obtained a theory of atomic structure, giving rise to the *Old Quantum Mechanics*. In 1919, during his last year at Manchester, he discovered that the nuclei of certain light elements, such as nitrogen, could be "disintegrated" by the impact of energetic alpha particles coming from some radioactive source, and that during this process fast protons were emitted. Blackett later proved, with the cloud chamber, that the nitrogen in this process was actually transformed into an oxygen isotope, so that Rutherford was the first to deliberately transmute one element into another. G. de Hevesy was also one of Rutherford's collaborators at Manchester. An inspiring leader of the Cavendish Laboratory, he steered numerous future Nobel Prize winners towards their great achievements: Chadwick, Blackett, Cockcroft and Walton. C.D. Ellis, his co-author in 1919 and 1930, pointed out "that the majority of the experiments at the Cavendish were really started by Rutherford's direct or indirect suggestion". He remained active and working to the very end of his life. Rutherford died in Cambridge on October 19, 1937. For more detailed biographical facts on Rutherford see the recent article online: *This Month in Physics History May, 1911: Rutherford and the Discovery of the Atomic Nucleus*, at the American Institute of Physics website: http://www.aps.org/publications/apsnews/200605/history.cfm

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Open problems about many-body Dirac operators

by Jan Dereziński (Warsaw, Poland)

Jan Dereziński studied physics at the University of Warsaw. He obtained his PhD in mathematics at Virginia Tech, Blacksburg USA, in 1985. His habilitation, defended in 1994 at the Faculty of Physics, University of Warsaw, was devoted to a proof of asymptotic completeness for the long-range N-body scattering. Since 2007 he is a full professor at the Faculty of Physics of University of Warsaw.
Research interests of J. Dereziński cover various aspects of quantum physics and quantum field theory, especially from the rigorous point of view. He is an author of a book "Scattering Theory of Classical and Quantum N-body Systems", written together with Christian Gérard. His new book "Mathematics of Quantization and Quantum Fields", also written together with C. Gérard, should appear soon in Cambridge Monographs on Mathematical Physics.

Recently, I exchanged a series of interesting email letters with a colleague from the Faculty of Chemistry, University of Warsaw, Prof. Bogumił Jeziorski. In these letters, Jeziorski formulated two interesting mathematical questions, which I would like to share with the readers of the Bulletin of the IAMP. Below, with the author's consent, I give an English translation of large parts of Jeziorski's letters.

> *Let us consider the essential self-adjointness of the Dirac-Coulomb operator H_{DC} for a helium-like ion. This operator has the form*
>
> $$H_{\mathrm{DC}} = D(1,Z) + D(2,Z) + 1/|\boldsymbol{r}_1 - \boldsymbol{r}_2|,$$
>
> *where*
>
> $$D(i,Z) := c\vec{\alpha}\vec{p}_i + m\beta - Z/|\boldsymbol{r}_i|,$$
>
> *$i = 1, 2$, is the usual Dirac operator for an electron i in a hydrogen-like ion of charge Z and $\boldsymbol{r}_i$, $i = 1, 2$, is the vector describing the position of the ith electron. (In the system of units used here, the speed of light c coincides with the inverse of the fine structure constant, $\alpha \approx 1/137.036$).*
>
> *It is well-known that the operator $D(i,Z)$ is essentially self-adjoint for $|Z| < \sqrt{3}/(2\alpha)$, although the Kato-Rellich Theorem proves this only for $|Z| < 1/(2\alpha)$. For $|Z| > \sqrt{3}/(2\alpha)$ there exist many self-adjoint extensions. For $|Z| < 1/\alpha$ there exists a distinguished self-adjoint extension, which can be adopted as the physical one [20].*
>
> *I think that adding $1/|\boldsymbol{r}_1 - \boldsymbol{r}_2|$ will not change the situation in an essential way and the Kato-Rellich Theorem will easily imply the essential self-adjointness of H_{DC}. Unfortunately, I was not able to find a proof of this statement in the*

> *mathematical literature. Perhaps, mathematicians view this as a rather easy generalization of Kato's proof for a nonrelativistic Helium atom.*
>
> *I believe the operator $H_{\rm DC}$ has a continuous spectrum from $-\infty$ to ∞. It would be very important to prove that there are no eigenvalues (corresponding to square integrable eigenfunctions) embedded in this continuous spectrum.*

I am not an expert in mathematical properties of many-body Dirac operators. There are a number of researchers (notably in Paris and Munich), who studied them and wrote interesting rigorous papers on this subject, such as [17, 3, 6]. However, I doubt whether a proof of either conjecture formulated in the letter of Jeziorski exists in the literature. I agree with him that these conjectures are plausible, interesting mathematically and well-motivated physically. They are well posed mathematically – they could be understood and appreciated even by a mathematician without a physical background.

The proof of the essential self-adjointness of the usual many-body Schrödinger operator with Coulomb interactions that I know [14] uses in an essential way the fact that the kinetic energy is quadratic in the momenta and is bounded from below. Dirac and many-body Dirac operators do not have these properties. Therefore, the usual proof of the essential self-adjointness does not generalize from the many-body Schrödinger to the many-body Dirac case. After discussing the problem briefly with some of my colleagues I realized that I even do not know how to prove the essential self-adjointness in the case $Z = 0$!

Our understanding of embedded point spectrum is even more limited. To my recollection, for many-body Schrödinger operators one can show the absence of positive eigenvalues [4] and the absence of embedded eigenvalues for generic localized interactions [1]. I do not know similar results for many-body Dirac operators. Let me quote again from a letter of Jeziorski.

> *Obviously, it would be more important to prove that $H_{\rm DC}$ has no eigenvalues* [than to show its essential self-adjointness]. *The Hamiltonian $H_{\rm DC}$ is used by chemists in hundreds of papers every year and with a tacit assumption that it has square integrable eigenfunctions. If one could prove that there are no such functions, I think that such a paper could be cited many times a year. I am somewhat surprised that mathematicians proved lots of difficult theorems on one-particle Dirac operators with singular potentials and, as it seems, were not interested in a system of two electrons with realistic potentials (...)*
>
> *If the singularity $1/|\boldsymbol{r}_i|$ is difficult, it could be regularized (which amounts to a finite nucleus model). If the singular nature of $1/|\boldsymbol{r}_1 - \boldsymbol{r}_2|$ causes problems, one could regularize this function as well, although this is much less justified physically. If such a regularization works and the resulting $H_{\rm DC}$ is easily shown to be essentially self-adjoint, it only remains to prove the absence of point spectrum. Perhaps this would work?*

A separate question arises: what is the physical relevance of many-body Dirac-Coulomb operators? To my understanding, many-body Dirac operators are postulated in chemistry and physics ad hoc, by analogy with many-body Schrödinger operators.

Many-body Schrödinger operators are well justified as Hamiltonians describing nonrelativistic matter. Note, in particular, that they are covariant with respect to the basic group of nonrelativistic physics – the Galilean group. It should be possible to derive many-body Schrödinger operators with Coulomb interactions as low-energy effective Hamiltonians from the full QED. (Of course, the full QED has well-known mathematical problems – it is believed to exist only as a perturbative theory. But this is another question).

The status of interacting many-body Dirac operators is much more shaky. They are not bounded from below, which indicates that they are not Hamiltonians of quantum dynamics. Unfortunately, they have another serious flaw: they are not covariant with respect to the Poincaré group. Perhaps, they describe approximately the time evolution of some time-ordered Green's functions. Maybe they appear in a certain natural approximate version of the Bethe-Salpeter equation.

Nonrelativistic many-body quantum mechanics is a difficult theory, but at least it is based on solid foundations – the many-body Schrödinger Hamiltonian. When one tries to generalize it to the relativistic setting, one seems essentially forced to adopt the point of view of quantum field theory. Unfortunately, the bound-state problem in quantum field theory is poorly understood.

There exists, however, a class of relativistic many-body problems where apparently a rather systematic and successful theory exists. This class includes few-body systems such as the positronium, hydrogen-like, helium-like, or even lithium-like ions. The most famous example of this category is the so-called Lamb shift. To my knowledge, there exist systematic perturbative methods to compute energy levels of such system. They always need a small parameter – usually the fine structure constant α, sometimes also $1/Z$ and the ratio of electron to nucleus mass. Non-perturbative QED is not known; probably it does not exist.

Note, however, that energy levels are not computed as eigenvalues of a self-adjoint Hamiltonian. They are defined as the position of the poles of Green's functions [11], or are derived from the adiabatic S-matrix formalism of Gell-Mann–Low [9]. In particular, they usually have a non-vanishing imaginary part describing the width of the resonance. Computations of few-particle relativistic energy levels are a specialty of another colleague of mine, Krzysztof Pachucki from the Institute of Theoretical Physics (Faculty of Physics, University of Warsaw). Pachucki taught me that systematic computations of these problems do not involve the many-body Dirac Hamiltonian, but rather the many-body Schrödinger Hamiltonian. Interesting examples of such results are contained in two recent papers by a group of researchers including Jeziorski and Pachucki [7, 13] devoted to molecular hydrogen, which is a few-body system, with 2 heavy and 2 light constituents. The analysis contained in these papers starts from a 4-body Schrödinger operator, with computations that go beyond the Born-Oppenheimer approximation and then include relativistic corrections. Jeziorski writes:

> *We are especially proud of Fig 3 in [7], which shows the QED effects in the molecular spectrum determined experimentally and their comparison with our theoretical prediction – first such observations in the literature.*

[Fig. 3 shows QED contributions to the rotational excitation energies of molecular hydrogen for the zero vibrational number – comparison of the theoretical calculations (open diamonds) with the experimental data. Almost all diamonds fall well inside the vertical bars denoting experimental uncertainties].

Let me quote again Jeziorski:

> *I would like to note that I am not involved in solving the Dirac-Coulomb equation. In our computations based on QED this equation does not appear. However, it is the foundation of the so-called "relativistic quantum chemistry", because the majority of chemists do not realize that it cannot have a pure point spectrum. In my opinion, it does not have a pure point spectrum, and its absence is beyond any doubt (Pachucki has the same opinion). On the other hand, chemists can say that since there is no mathematical proof, they can have doubts! There exists, however, strong numerical evidence – the so-called Brown-Ravenhall disease (BRD) [2], called also the "continuum dissolution", and three papers from Jacek Karwowski's group in Toruń [12], where for the first time the width of the resonance modeling the ground state of the helium atom was computed. As a proof of the strength of the faith in the existence of eigenvalues of the Dirac-Coulomb Hamiltonian let me mention that in a recent monograph [15] one can find a statement "continuum dissolution has never been observed in actual calculations". Another influential monograph [5] views the destructive effect of BRD as only "alleged". It should be mentioned, however, that the significance of the results of Refs. [12] has been recently noticed in the chemical literature [8].*

I am greatly surprised that the belief in the existence of embedded point spectrum of Dirac-Coulomb operators is so widespread. I have always thought that every physicist or mathematician who played a little with the perturbation theory for operators has developed the intuition that embedded eigenvalues are an exceptional, non-generic phenomenon that needs special circumstances to happen. (This does not mean that it should be easy to prove their absence in concrete situations).

Jeziorski sent me a very recent review paper [10] of Wenjian Liu, an authority in relativistic quantum chemistry, suggesting to read page 4 of this paper. It appears that Liu does not believe that the DC equation has no eigenvalues. Liu discusses the results of [12], trying to find a flaw in it. Here is an excerpt of Liu's paper:

> *Therefore, it cannot be excluded that the the complex energies obtained by Pestka et al [12] are due to incompleteness errors in the basis set. Given such uncertainties, the conclusion that the DC Hamiltonian has no bound states may be premature. What can really be concluded at this stage is that the BRD is much less virulent than originally claimed, and that the no-pair projection, as recommended by Sucher, for avoiding the BRD, is not really needed.*

The many-body Dirac equation is used by many chemists. Apparently, they have some success in predicting properties of atoms and molecules. Here again a comment of Jeziorski:

> *They* [chemists that use the Dirac-Coulomb equation] *obtain good numbers, because for heavy atoms the Dirac-Coulomb model is much better than the Schrödinger model, in spite of its artifacts. This is because the widths of resonances of the DC equation (which model bound states) are apparently of the order of $Z^3\alpha^3$, and the relativistic corrections from DC equation scale as $Z^4\alpha^2$* [both relative to the nonrelativistic energy $m\alpha^2$.] *The ratio of the (non-physical) resonance width to the relativistic correction is therefore α/Z. Additionally, the error involved in solving the DC equation, which amounts to finding the resonances, is much bigger than their width. Most cases of the agreement with experiments belong to structural chemistry and thermochemistry, where experimental errors are much bigger than $Z^3\alpha^3$ (but often smaller than $Z^4\alpha^2$).*

Sometimes it is claimed [19] that in quantum chemistry one should not use the many-body Dirac operator itself, but its compression $PH_{\rm DC}P$, where

$$P = P_1 \otimes P_2 \ldots \otimes P_N,$$

N is the number of electrons and P_i is the orthogonal projection onto one-electron states of "positive energy". The advantage of the "Sucher's no-pair Hamiltonian" $PH_{\rm DC}P$ is its boundedness from below. However, in order to determine the projections P_i one needs to adopt a certain 1-electron potential, which is to a large extent arbitrary. In practice, the operators $PH_{\rm DC}P$ seem to be mostly used in intermediate steps when eigenvalues of the unprojected operator $H_{\rm DC}$ are computed.

Anyway, together with Jeziorski, I believe that, most likely, what chemists compute are not true eigenvalues of the many-body Dirac-Coulomb operator, but its resonances. This leads to a nontrivial question what is a mathematical definition of a resonance.

There exists a satisfactory definition of a resonance for many-body Schrödinger operators. As it is well-known, they are eigenvalues of the operator distorted by dilation analyticity. Equivalently, they can be defined as poles of the resolvent between dilation analytic vectors.

For one-body Dirac-Coulomb operators the dilation analyticty approach goes through [21, 16]. For many-body Dirac-Coulomb operators apparently it is difficult to apply this approach rigorously [18], even though it is used in numerical studies in the 2-body case in [12].

Thus, there are two problems that I do not understand. Unfortunately, these problems are quite vague – they are not as rigorously formulated as Jeziorski's questions.
– What is a good definition of a resonance for many-body Dirac-Coulomb operators?
– What is a physical justification (that essentially means, a derivation from QED) of applications of many-body Dirac-Coulomb operators to atoms and molecules?

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Mathematical analysis of complex networks and databases

by Ph. Blanchard & D. Volchenkov (Bielefeld, Germany)

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Use Random Walks to Reveal System Properties

Most of the networks and databases humans have deal with contain a large albeit finite number of units. Their structure maintaining functional consistency of the components is essentially not random and calls for a precise quantitative description of relations between nodes or data units and all network parts, as having important implications for the network robustness. A network can be seen as a discrete-time dynamical system possessing a finite number of states (nodes). The behavior of such a dynamical system can be studied by means of a transfer operator which describes the time evolution of distributions in phase space. The transfer operator can be represented by a stochastic matrix determining a discrete time random walk on the graph, in which a walker picks at each node between the various available edges with equal probability. An obvious benefit for graph theory of the approach based on random walks is that the relations between individual nodes and subgraphs acquire a clear and detailed probabilistic description that enables us to attack applied problems which could not even be started otherwise. In contrast to classical graph theory paying attention to the shortest paths of least cost, in the probabilistic approach developed in [1, 2, 3], all possible paths between a pair of vertices in a connected graph or a pair of units in a database are taken into account, although some paths shall be more probable than others. In such a formulation of graph theory, the distance is nothing else than a "path integral". In analogy with quantum mechanics, where the wave functions of multi-fermionic systems satisfying the Pauli exclusion principle are approximated by the Slater determinants, the squared determinants over the

elements of eigenvectors of the transition matrix provide us with the probability amplitudes over all subsets of nodes and transition modes. The Laplace operator associated to random walks possesses a group generalized inverse that can be used in order to define a probabilistic Riemannian manifold with a random metric on any finite connected undirected graph. Each node of the graph is characterized by a vector the squared norm of which is nothing else but the first passage time to the node, the expected number of steps required to reach the node for the first time starting from a node randomly chosen among all nodes of the graph accordingly to the stationary distribution of random walks. The distance between any two nodes of the graph, x_1 and x_2, is given by the commute time of random walks between them, defined as the expected number of steps taken by a random walker starting from x_1 to reach x_2 and subsequently return to x_1. These characteristic times describing the first encounter properties of the random walk remain finite even for a directed graph, although it lacks the Euclidean space structure. Random walks defined on connected undirected graphs have a deep connection to electric resistor networks. The effective resistance between two nodes of an electric resistor network, defined as the potential difference between them at a unit current, is equal (up to a normalization) to the commute time of a random walk between them. The effective resistance distance is bounded above by the shortest path distance and equals the shortest path distance only if the graph forms a tree, in which any two nodes are connected by the only possible path.

In [2, 3], we applied the probabilistic approach for the analysis of urban structures, evolution of languages and musical compositions. In particular we demonstrate that random walks and diffusions defined on spatial city graphs might spot hidden areas of geographical isolation in the urban landscape going downhill. The first passage time to a place correlates with the assessed value of land in that. The method accounting the average number of random turns at junctions on the way to reach any particular place in the city from various starting points could be used to identify isolated neighborhoods in big cities with a complex web of roads, walkways and public transport systems.

Geometric Representations of Language Taxonomies

Many language groups had originated after the decline and fragmentation of territorially-extreme polities and in the course of migrations when dialects diverged within each local area and eventually evolved into individual languages in an extremely complex process of permanent interactions with other languages that reflects a genuine higher order influence among the different language groups. Generally speaking, the number of parameters describing all possible parallels we may observe between the linguistic data would increase exponentially with the data sample size. The only hope to perform any useful data analysis in such a case relies upon a proper choice of features that re-expresses the data set to make all contributions from an asymptotically infinite number of parameters convergent to some non-parametric kernel. While comparing two words, w_1 and w_2, we use [4] the edit distance divided by the number of characters of the longer of the two, $D(w_1, w_2) = \|w_1, w_2\| / \max(|w_1|, |w_2|)$ where $\|w_1, w_2\|$ is the standard edit distance accounting for the minimal number of insertions, deletions, or substitutions of single letters needed to transform the word w_1 into w_2, and $|w|$ is the number of

characters in the word w. For example, the normalized edit distance between the orthographic realizations of the meaning *milk* in English and in German (*Milch*) equals 2/5. In order to obtain the lexical distances between the two languages, l_1 and l_2, we compute the average of the above distances over Swadesh's vocabulary [5] of 200 meanings essentially resistant to changes - the smaller the result is, the more affine are the languages, $d(l_1, l_2) = \sum_{\alpha=1...200} D\left(w_\alpha^{(l_1)}, w_\alpha^{(l_2)}\right)/200$, where α is a meaning from Swadesh's vocabulary, and $w_\alpha^{(l)}$ is its orthographic realization in the language l. A random walk associated to the matrix of lexical distances $d(l_i, l_j)$ calculated over the Swadesh vocabulary for a sample of N different languages is defined by the transition probabilities $T(l_i, l_j) = \Delta^{-1} d(l_i, l_j)$ where the diagonal matrix $\Delta = \mathrm{diag}(\delta_{l_1}, \delta_{d_2}, \ldots \delta_{l_N})$ contains the cumulative lexical distances $\delta_{l_i} = \sum_{j=1}^{N} d(l_i, l_j)$, for each language l_i. Random walks ascribe the total probability of successful classification for any two languages in the language family, $P(l_i, l_j) = \lim_{n\to\infty} \sum_{k=0}^{n} T^k(l_i, l_j) = L^{-1}$. The latter operator is the generalized inverse of the Laplace operator $L = \mathbf{1} - T$. Each diagonal element of L^{-1} of the above kernel is the first-passage time of random walks to a language defined on the weighted undirected graph determined by the matrix of lexical distances $d(l_i, l_j)$, and the off-diagonal entries quantify the interference of two random walks concluding at l_i and l_j respectively. The kernel L^{-1} plays the same role for the structural component analysis, as the covariance matrix does for the usual principal component analysis. The eigenvectors of L^{-1} define an orthonormal basis in $\mathbb{R}^N$ which specifies each language l_i by N numerical coordinates, $l_i \to (q_{1,i}, q_{2,i}, \ldots q_{N,i})$, which are the signed distances from the point representing the language l_i to the axes associated to the virtually independent components. Languages that cast in the same mould in accordance with the N individual data features are revealed by geometric proximity in Euclidean space spanned by the eigenvectors $\{q_k\}$ that might be either exploited visually, or accounted analytically. The rank-ordering of data traits $\{q_k\}$, in accordance to their eigenvalues $0 = \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_N$, provides us with the natural geometric framework for dimensionality reduction.

The principal components of the Indo-European (IE) family reveal themselves in Fig. 1 by four well-separated spines representing the four biggest traditional IE language groups: Romance & Celtic, Germanic, Balto-Slavic, and Indo-Iranian. These groups are monophyletic and supported by the sharply localized distributions of the azimuth and inclination (zenith) angles over the languages. It is remarkable that the division of IE languages with respect to the azimuthal and zenith angles evident from the geometric representation perfectly coincides with the well-known *centum-satem* isogloss of the IE language family (the terms are the reflexes of the IE numeral '100'), related to the evolution in the phonetically unstable palatovelar order. The colonization of the Pacific Islands is still a recalcitrant problem in the history of human migrations, despite many explanatory models based on linguistic, genetic, and archaeological evidences have been proposed in so far. The components probe for a sample of 50 Austronesian (AU) languages immediately uncovers the both Formosan (F) and Malayo-Polynesian (MP) branches of the entire language family (see Fig. 2). The distribution of azimuth angles identifies them as two monophyletic jets of languages that cast along either axis spanning the entire family plane. The clear geographic patterning is perhaps the most remarkable aspect of the

geometric representation.

In [4], the derived geometric representations of language taxonomies are used in order to test various statistical hypotheses about the evolution of languages. Our method allows for making accurate inferences on the most significant events of human history by tracking changes in language families through time.

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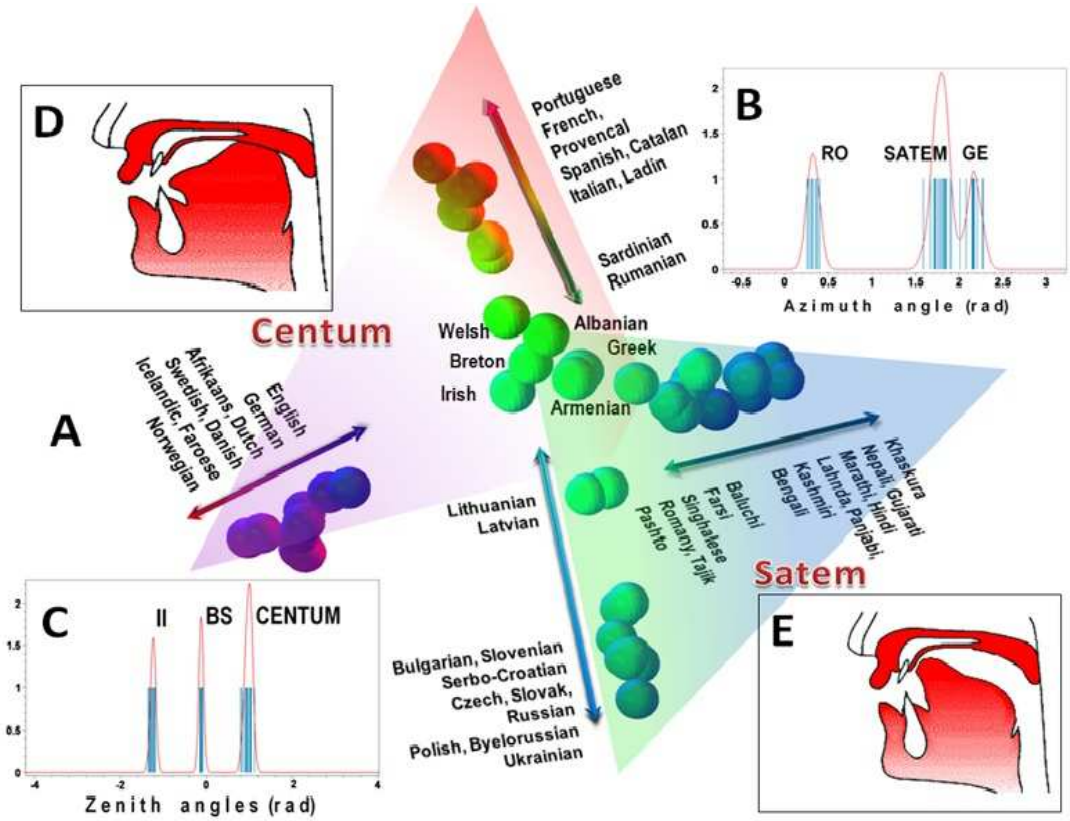

Figure 1: (**A**) The three-dimensional geometric representation of the IE language family in space of the major data traits (q_2, q_3, q_4) color coded. Due to the central symmetry of representation, it is convenient to use the spherical coordinates to identify the positions of languages: the distance from the center of the graph, the inclination angle, and the azimuth angle. (**B**). The kernel density estimates of the distributions of azimuthal angles in the three-dimensional geometric representation of 50 languages of the IE language family, together with the absolute data frequencies. Romance (RO), Germanic (GE), and the satem languages (SATEM) are easily differentiated with respect to the azimuthal angles. (**C**). The kernel density estimates of the distributions of inclination (zenith) angles in the three-dimensional geometric representation of 50 languages of the IE language family, together with the absolute data frequencies. Indo-Iranian (II), Balto-Slavic (BS), and the centum languages (CENTUM) are attested by the inclination (zenith) angles. The palatovelar sounds merge with the velars in centum languages (**D**) sharing the azimuth angle, while in satem languages observed at the same zenith angle the palatovelars shift to affricates and spirants (**E**).

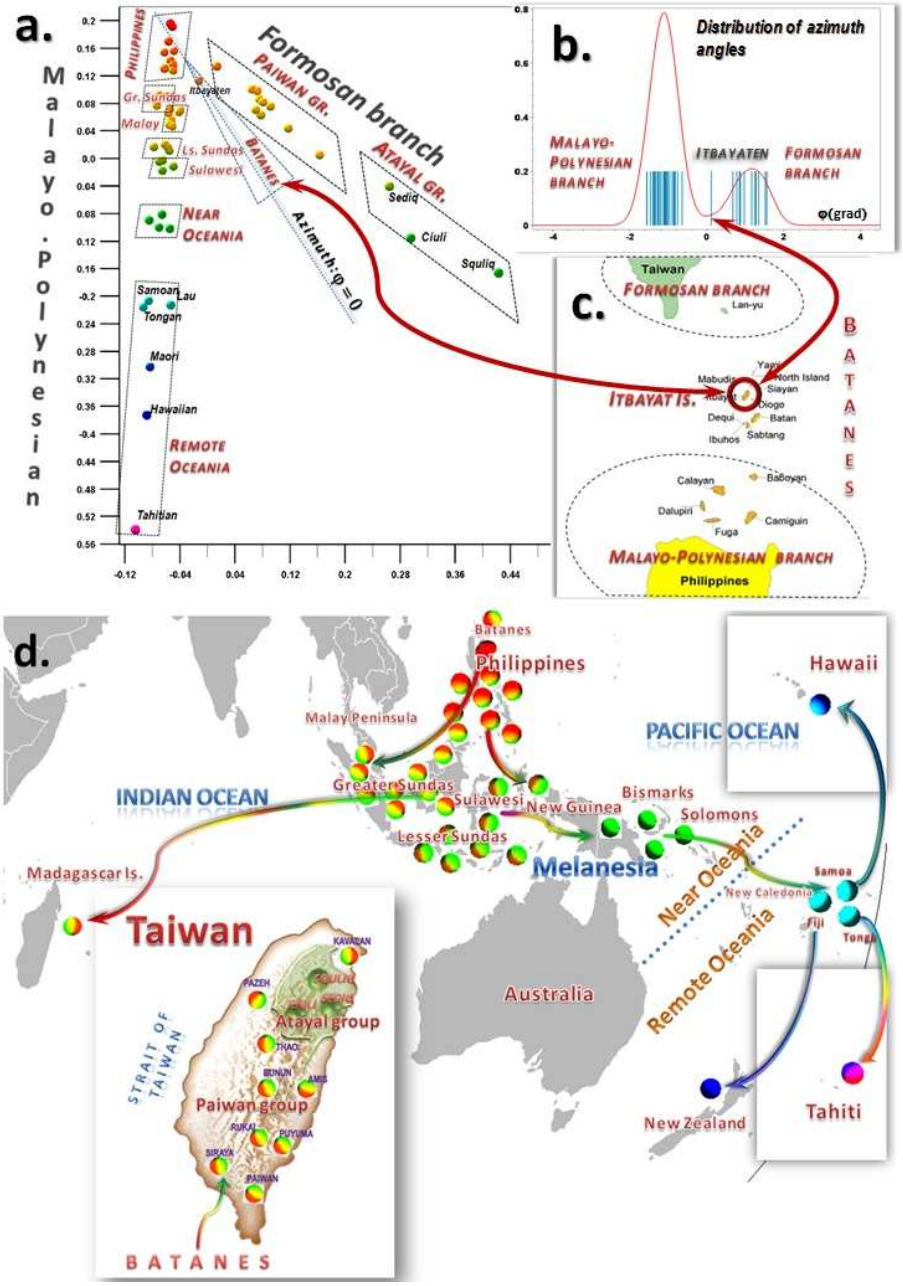

Figure 2: (**a**) The geometric representation of the 50 AU languages in space of the major data traits (q_2, q_3) shows a remarkable geographic patterning. It is convenient to use the polar coordinates: the distance from the center of the graph, $r_i = \sqrt{q_{2,i}^2 + q_{3,i}^2}$, and the azimuth angle $\varphi = \arctan\left(\frac{q_{3,i}}{q_{2,i}}\right)$, to identify the positions of languages. (**b**) The distribution of azimuth angles in the geometric representation of the 50 AU languages. (**c**) The Itbayaten language is pretty close to the azimuth, $\varphi = 0$, bridging over the language family branches lexically and geographically. (**d**) The geometric representation of the 50 AU languages projected onto the geographic map uncovers the possible route of Austronesian migrations.

ICMP12 News

Below is a summary of the information on the XVIIth International Congress on Mathematical Physics (ICMP12). Always use the conference web site www.icmp12.com to get updated information.

- Plenary speakers are announced.
- Topical session speakers will be announced early February 2012.
- Contributed talks are not yet accepted. Information on both the submission procedure and the selection procedure will be available February 15, 2012.
- Registration is now open! Go to

  www.icmp12.com/registration.aspx.
- Information on flights to Aalborg can be found at

  www.icmp12.com/travel-information.aspx
- Information on accommodation can be found at

  www.icmp12.com/accommodation.aspx.

  For those that travel by car we would like to draw your attention to the last part concerning rental of a holiday home.
- Application for Congress Fellowships are accepted. **Deadline March 15, 2012.**

  Note that there are two categories: Fellowships for participants from less favored regions, and NSF support for younger US based participants.

Visa information: If you need a visa to participate in the Congress, read carefully the visa information section at
www.icmp12.com/visa-information.aspx
and follow the instructions. It is important to apply EARLY!

Congress poster. The congress poster is available for download at
www.icmp12.com/poster-download.aspx

You are encouraged to print and display it. A number of printed copies will be mailed to institutions etc.

We look forward to seeing all IAMP members in Aalborg for the ICMP12. Do not forget the Young Researcher Symposium, August 3–4, 2012, preceding the ICMP12! Also do not forget

Prizes! The recipients of

- The Henri Poincaré Prize
- The IAMP Early Career Award
- The IUPAP Young Scientist Award in Mathematical Physics

will be announced at the beginning of the Congress, Monday August 6, and the prizes awarded in a ceremony that day.

PhD course. A PhD course on various topics of Mathematical Physics intended as a warm-up for ICMP12 will take place in Aalborg on May 2-3, 2012. A detailed description can be found here: http://www.icmp12.com/satellite-meetings/phd-course-%27topics-in-mathematical-physics%27.aspx

Arne Jensen (Congress Convenor)

NSF support for ICMP participants

US National Science Foundation
support for young researchers at US institutions
for the XVIIth International Conference on Mathematical Physics
and Young Researchers Symposium,
Aalborg, Denmark, 3-4 and 6–11 August 2012

Funding is anticipated from the US National Science Foundation for a block grant to support the participation of young researchers at US institutions in the XVIIth International Congress on Mathematical Physics and the Young Researchers Symposium both to be held in Aalborg, Denmark, during the period 3–11 August 2012. This grant will provide support for travel, lodging, and local expenses. Applicants must have a position (graduate student, post-doc or assistant professor) at a US institution and be not more than 5 years beyond the PhD. Preference will be given to those without other sources of funding. Co-funding from an applicant's institution is encouraged. Women and members of under-represented groups are especially encouraged to apply.

Deadline for applications is 15 March 2012. Announcements of awards will be made by 15 April 2012. Applications and questions should be sent to Peter Hislop at icmp2012@hotmail.com. Additional information and application procedure can be found at:

http://www.ms.uky.edu/~hislop/icmp2012.html

Peter Hislop (Kentucky, USA)

News from the IAMP Executive Committee

New individual members

IAMP welcomes the following new members

1. Joachim Asch, Centre de Physique Théorique, Université du Sud Toulon Var, France
2. Diana Barseghyan, Department of Theoretical Physics, Academy of Sciences of the Czech Republic, Rež, Czech Republic
3. Pangiatos Batakidis, Mathematics Department, University of Cyprus, Nicosia, Cyprus
4. Paul Bourgade, Mathematics Department, Harvard University, Cambridge MA, USA
5. Francis Brown, Institut de Mathématiques de Jussieu, Paris, France
6. Wojciech Dybalski, Zentrum Mathematik, TU München, Garching, Germany
7. Sabine Jansen, Weierstrass-Institut für angewandte Analysis und Stochastik, Berlin, Germany
8. Douglas Lundholm, Forschungsinstitut für Mathematik, ETH Zürich, Switzerland
9. Bernard Clark Musselman II, Mathematics Department, Michigan State University, Lansing MI, USA
10. Alexander Nikolaevich Pechen, Steklov Institute for Mathematical Sciences, Russian Academy of Sciences, Moscow, Russia
11. Miloud Rahmoune, Physics Department, Moulay Ismail University, Meknes, Morocco
12. Alexei Rebenko, Institute of Mathematics, National Academy of Sciences of Ukraine, Kiev, Ukraine

Recent conference announcements

Operator Theory and Mathematical Physics (OTAMP)
June 11–14, 2012, Centre de Recerca Matemàtica (CRM), Barcelona, Spain

http://www.crm.cat/Activitats/Activitats/2011-2012/OTAMP/web-otamp/

This conference is supported by the IAMP.

Open positions

Post-doctoral position in mathematical physics

The Mathematical Physics group at the Helsinki University

http://wiki.helsinki.fi/display/mathphys/Home

is seeking a post-doctoral researcher in the field of non-equilibrium statistical mechanics. The position is funded through a European Research Council (ERC) Advanced Grant and will be up to 3 years. The researcher will be working in an active research environment including the Center of Excellence in Analysis and Dynamics. Applicants should send a CV and three letters of recommendation by email to antti.kupiainen@helsinki.fi. Deadline for application is January 31, 2012 , and the position will be available September 1, 2012. An earlier start date is also possible.

PhD Position

Duration: 3 years, starting in Fall 2012
Location: University of Cergy-Pontoise, France
Salary: approx. 1 450 (no teaching) / 1 700 (with small teaching duty), after taxes, per month on 12 months.

The candidate should have a good background in spectral theory, nonlinear analysis and PDEs, or numerical analysis. He is expected to work on subjects related to the ERC project *Mathematics and Numerics of Infinite Quantum Systems*, see

http://mniqs.math.cnrs.fr.

To apply, please send a CV to mathieu.lewin@math.cnrs.fr.

New open positions are also announced on the IAMP webpage

http://www.iamp.org/page.php?page=page_positions

Manfred Salmhofer (IAMP Secretary)