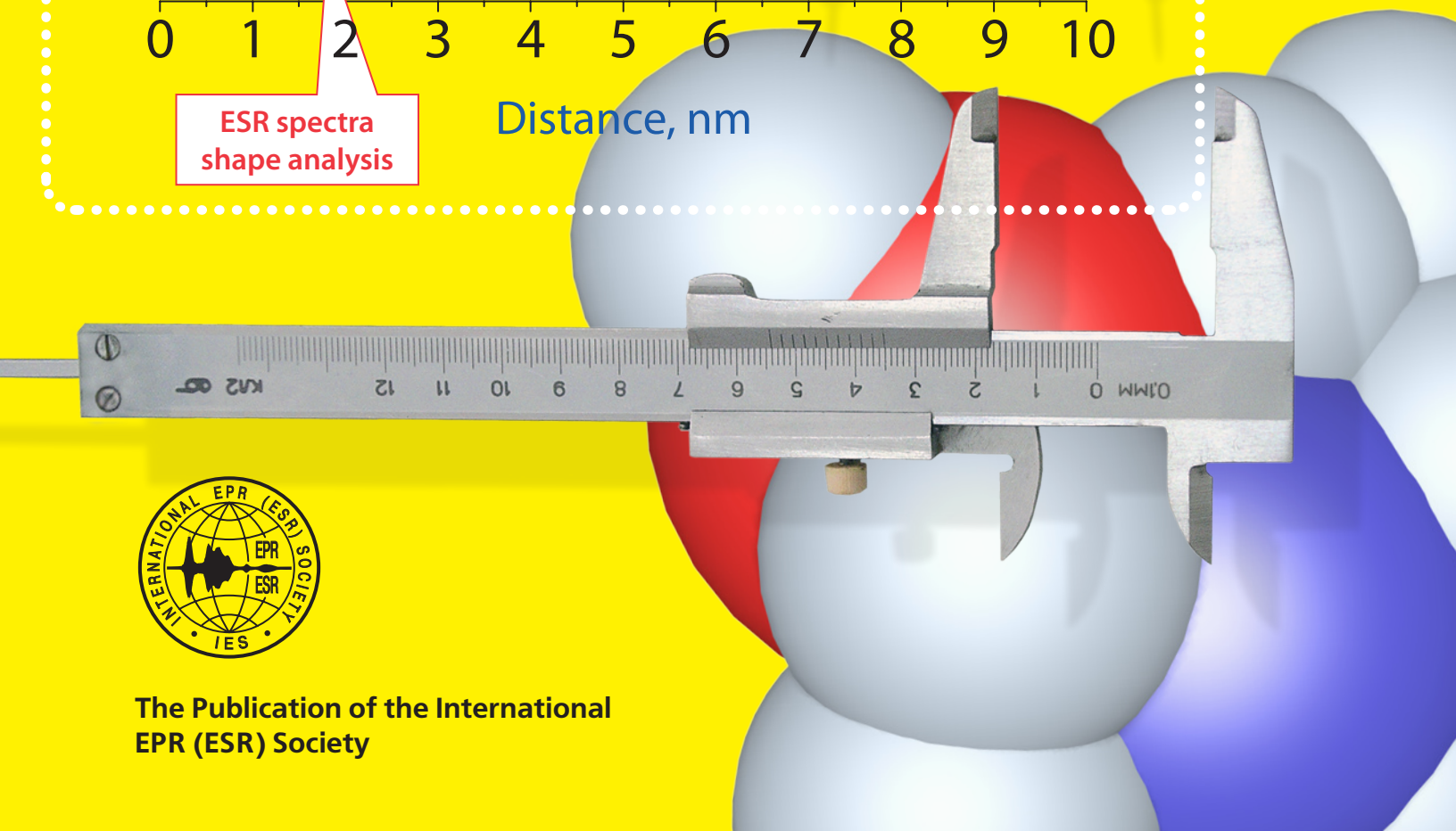
epr newsletter

2007
volume 17 number 1



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Please feel free to contact us with items (news, notices, technical notes, and comments) or ideas for the *EPR newsletter*.

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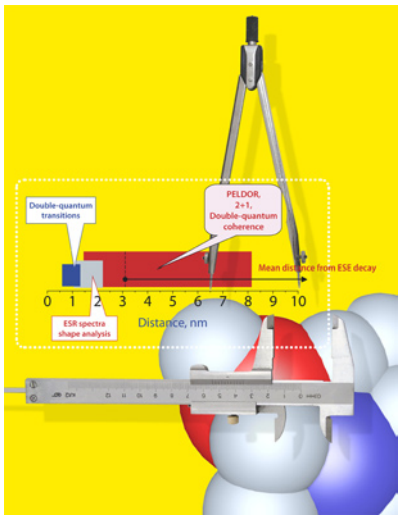

The cover picture illustrates aspects of research carried out by Yurii D. Tsvetkov, recipient of the Bruker Prize 2006. It shows the distance range which can be measured by some continuous-wave and pulsed EPR/ESR methods.

epr newsletter

The Publication of the International EPR (ESR) Society

volume 17 number 1 2007

ETH
Eidgenössische Technische Hochschule Zürich
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Editorial

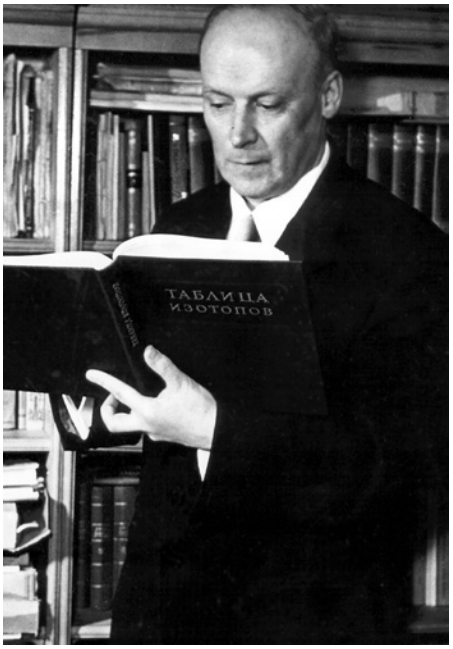
Dear colleagues,

As you perused the 'Notices of Meetings' column in the previous issue (16/4, p. 20) you may have noticed the announcement regarding the International conference "Modern Development of Magnetic Resonance" (Zavoisky100), marking the 100th birthday of Evgeny Konstantinovich Zavoisky, the pioneer of electron paramagnetic resonance.

We have published several articles concerning E. K. Zavoisky which include an interview with his daughter, Nataliya E. Zavoiskaya (13/1-2, pp. 13–14), a story about his passion for modern painting (14/4, pp. 6–7) and a story about the discovery of EPR by E. K. Zavoisky (14/4, pp. 12–13). Nataliya E. Zavoiskaya emphasized that her father never stopped his EPR activity, meeting with his EPR colleagues and discussing relevant problems. As a young student, I had seen Prof. Zavoisky at a seminar in the Kazan Physical-Technical Institute during one of his last visits to Kazan. The many years that have passed since then have erased the contents of this seminar from my memory, but I still remember his soft voice and very unaffected manner. Yes, you can always tell a great man by his manner – never pompous!

It is wonderful to meet people in person. It enriches you with the understanding of their personality and you always learn something.

In 2005, I met Gary Gerfen at the 28th International EPR Symposium in Denver. During one of the coffee breaks he told me that he had notes written by Bill Mims on the first days of electron spin echo spectroscopy in biology, and Gary wondered if I might be interested in publishing them in the EPR newsletter. He gave me a file with these pages, and I skipped one session of the EPR symposium in order to read it. Gosh, it was something to read! You immediately get the feeling of being an insider and of how the research in this field developed from the very first experiments. I told Gary we would be happy to publish this article in the 'EPR newsletter Anecdotes' column and that he should contact John Pilbrow who edits this column. John approved of this article to be published, but the only problem was that the article was quite long.



E. K. Zavoisky (1907–1976)

Gary and John did not like the idea of publishing a shortened version: Bill Mims' reminiscences were worthy of publication in their entirety. The only solution was to divide the notes into three articles and in this issue you are privileged to read Part I (p. 10). Parts II and III will follow in the *newsletter* 17/2 and 17/3, respectively. I am grateful to Gary and John for all their efforts. The photo of Bill Mims illustrating this article was taken in Kazan in 1991 when Bill came there to get his Zavoisky Award. It was the first Zavoisky Award celebration and Bill came there only for one day. A large group of the participants of the ISMAR Workshop on Electron Spin Echo Spectroscopy (Novosibirsk, September 25–28, 1991) joined the celebration to congratulate Bill Mims on his award.

After meeting Alex I. Smirnov, the recipient of the IES Young Investigator Award 1998, at several conferences, only in his article "From Russia with EPR" (p. 4) I learned that he was an undergraduate and then a graduate student of Yakov S. Lebedev. His article shows vividly the working atmosphere in Lebedev's group, in particular, the importance of scientific freedom.

It was an interesting story with the article "A Passion for Wrestling" by Dave Thomas. Last year Dave came to Kazan to participate in the International conference "Modern Development of Magnetic Resonance" timed to the Zavoisky Award 2006 celebration. One of the first questions he asked me was if there could be an option for him to swim in the river Volga. Was I not surprised? It was the end of September and local people stop swimming in the river Volga already in the end of August because it becomes too cold to swim. However, during our after-conference trip to the Raifa monastery we came to our greatest river and Dave bravely stepped into its icy cold waters. The rest of the group watched him standing under umbrellas in their warm jackets. He was met with a storm of applause when he finished his swimming. He also mentioned his wrestling experience and I thought it was a perfect subject for the 'Another Passion' column. You have one guess that I have immediately started my attack on Dave but he was quite reluctant to write this article. To make a long story short, you find Dave's article on p. 6, which means that in this psychological "wrestling" he was a perfect gentleman and let a lady win.

The article by John Weil in the 'Tips and Techniques' column (p. 13) underlines the importance of understanding what the notion "tensor" widely used in radiospectroscopy means in reality. Please pay special attention to the announcement about the second edition of the book "Electron Paramagnetic Resonance: Elementary Theory and Practical Applications" by J. A. Weil and J. R. Bolton (p. 14), in which this subject is dealt with in detail. Hope that in the forthcoming issues of the newsletter we will have such educational articles on a regular basis. Interestingly enough, it was at the 29th EPR Symposium in Breckenridge in 2006 where John gave me the first draft of this article. In the meantime he continued working on it and the final version shows how our great scientists work on their papers, carefully choosing the right word in the right place.

Back to a very important subject – paying membership dues. At present there is a convenient option to pay them by visiting the IES website. If you already paid them, good for you and us! If not, please do that. Thank you!

Laila Mosina

Are you interested to become a member of the International EPR (ESR) Society? Please find the registration/information form for new/continuing members of the IES and non-credit-card payment instructions for individual members on this Web site: www.epr-newsletter.ethz.ch/contact.html

Fellowship of the IES to...

Professor Les H. Sutcliffe

FELLOW OF THE SOCIETY 2007

Wolfgang Lubitz (left) and Les Sutcliffe (right). New College, Oxford, UK, March 26, 2007.

Professor Les Sutcliffe is a pioneer magnetic resonance spectroscopist. He obtained his B.Sc. at the University of London and his Ph.D at the University of Leeds. His initial researches were in chemical kinetics using optical spectroscopy. He was one of the first British scientists to install both EPR and NMR spectrometers in his laboratory. Thereafter, he has applied himself almost equally to EPR spectroscopy and NMR spectroscopy, combining them whenever possible. He has carried out his researches at the University of Liverpool, Royal Holloway College (University of London), the University of Surrey and the Institute of Food Research (Norwich).

Les is appointed a Fellow of the International EPR/ESR Society in recognition of his outstanding contributions to EPR spectroscopy including his discoveries of new classes of sulphur-nitrogen containing heterocyclic free radicals; the design and synthesis of new stable aromatic nitroxides and exploitation of them as spin probes; EPR and NMR spectroscopy of cation radicals derived from chromanols; spin trapping. Les has, with D. G. Gillies, been involved in the construction of two 300 MHz EPR imagers based on NMR technology.

Apart from a publication record of over 200 refereed papers, Les is a co-author of a classic two-volume monograph "High Resolution Nuclear Magnetic Resonance Spectroscopy" which he wrote with his collaborators J. W. Emsley and J. Feeney. He is also founder and a co-editor of the review series "Progress in Nuclear Magnetic Resonance Spectroscopy" which is now in its 50th volume. Les has supervised over 50 doctoral students and a notable feature of his career is the high level of international collaboration.

The title of Fellow of the Society is conferred on those who have made truly outstanding contributions to EPR theory and/or practice. It is very appropriate that Les Sutcliffe should be honoured with a Fellowship of the International EPR/ESR Society.

IES Young Investigator Award Revisited

This column features former recipients of the IES Young Investigator Award.

From Russia with EPR

I first entered an EPR lab as a fourth year student of the Moscow Institute of Physics and Technology. The lab I have chosen for my research project was headed by Professor Yakov Lebedev and was located in Building #1 of the Moscow Institute of Chemical Physics of the Soviet Academy of Sciences. The building was old but the setting was simply spectacular. It overlooked the entire downtown Moscow from the top bank of the Moscow river. What else could it be for the former summer residence of the vice-governor of Moscow built during czar time! But even more fantastic were the people working in the lab and the Institute at that time.

The first project assigned to me was to develop two-dimensional (2-D) EPR imaging. During our initial meeting, Professor Lebedev told me that his group was already collecting 1-D data on the distribution of paramagnetic species along the direction of the magnetic field gradient and that the next step should be reconstructing a 2-D image, something that just recently had been demonstrated by Larry Berliner and Hirotada Fujii (Science, 227: 517–519 (1985)). At that time I knew very little about EPR but even less about image reconstruction from projections. Frankly, I knew absolutely nothing about the latter. But the project sounded rather interesting and the next day I headed for the library. At that pre-internet time, the literature search had a very different meaning: one had to actually go to the library, open the catalog drawers, walk into the book stacks to pull out the journals, and then do all this over again while 'chasing' articles from obscure sources. This chase was not as thrilling as uncovering the DaVinci code in a recent bestseller, but I remember traveling all over Moscow to get to a certain library depository and find the only copy of IEEE Communications in the entire city, and, possibly, even Russia. The whole thing was also very time consuming: it took me quite a few weeks to learn the back projection algorithm and how to program a code that would fit into the memory of an old computer. Several years later, on the day I defended my PhD thesis, Prof. Lebedev told me that after he did not see me in a lab for about a month he started to worry quite naturally that, perhaps, I would never come again and that he would have to look for another student for this project. He also told me that during my first year in his lab he was not sure what I was actually working on.

All that happened much later. At the beginning of my EPR imaging project, nothing worked fine. For example, I had to reject several reconstruction algorithms I tried. Finally, after my program was debugged and working fine (on synthetic data), Prof. Lebedev told me that, perhaps, I should learn how to record an actual EPR spectrum. He reminded me that I am in a spectroscopy lab and that everyone should know at least how to tune an EPR spectrometer. This was indeed very useful and I have taken many, many spectra since then.

At that time, the Lebedev's group consisted of several subgroups, each involved in different projects: EPR imaging, FT EPR, high field EPR, and a couple of other studies. While my project as an undergraduate and then a graduate student was EPR imaging, I was still given a lot of freedom to interact with other subgroups. In fact, my advisor encouraged such interactions and was very pleased to see me publishing papers on other subjects. That is how I first got involved with high field EPR. The idea was to try EPR imaging at 130 GHz to take advantage of the exceptional sensitivity to limited volume samples. At one point of during that project we had to move data from one computer to another: we have accomplished this with the help of two senior researchers who hand-carried the entire fixed disk drive down the hallway. The effort paid off as a first paper on EPR imaging at high magnetic fields that appeared in J. Magn. Reson.

I was also encouraged to collaborate with plant biologists from Moscow State University. This is how I first learned about the fascinating role of lipids and lipid bilayers in biophysics – one of the main focuses of my laboratory at NCState today. One thing I remember is that I never had regular meetings scheduled with my advisor nor was told directly what to do on a daily/weekly basis. However, I could always walk into Prof. Lebedev's office and ask questions. My fellow students in the lab and senior colleagues were also of indispensable help. The most enlightening scientific meetings occurred during informal coffee breaks we had on regular basis in a small dark hallway before the main lab. Overall, I think by being given a significant amount of scientific freedom during my student years I was simply trusted to do my very best in research. This strategy paid off: my graduate and undergraduate work resulted in 16 peer-reviewed papers. It also gave me the very first taste of being, at least in a few aspects, an independent researcher, but, of course, having very little of today's responsibilities.

Today, in my laboratory at NCState I also like to give my PhD students and postdoctoral researchers a rather large degree of freedom. There are also so many things to do in magnetic resonance and EPR – from spintronics and, particularly, non-volatile magnetic memory to electrostatic and hydrogen bonding interactions in membrane protein systems. Even more exciting is to make the most of advances in nanoscience for manipulating biological self-assembly at nanoscale levels and to exploit an organic chemistry toolbox to make a series of EPR probes that would mimic natural amino acids. The only way I can pursue this research is through interdisciplinary collaboration and working with students and postdocs of very different backgrounds. Of course, I like the members of my group to succeed in pursuing research goals that I (and, hopefully our peer-reviewers) believe to be important. But what I like even more is when my students are trying the experiments I did not think of. I also like to learn from my students.

Alex I. Smirnov
North Carolina State University

Another Passion

A Passion for Wrestling

Dave Thomas

My passion for EPR began two decades after my passion for wrestling. I was born into a wrestling family. My father Dale and mother Nina were both Assistant Professors of Physical Education at Michigan State University. They met and married in 1948, and my twin brother Ken and I were born in 1949, followed by my brother Steve in 1950. We were instructed in wrestling before walking. In 1952 my father represented USA in the Helsinki Olympic games, and promotional photos were taken of him with his three wrestling babies, still in diapers (see photo 1). He was in graduate school at the time, working on his PhD in physical education, based on muscle mechanics. He placed fifth in Greco Roman wrestling in 1956 in Melbourne, just after he became Professor and wrestling coach at Oregon State University.

My first official wrestling competition was in 1957, when I was 8 years old. That year my father started the nation's first Kid Wrestling program, starting with boys in my Cub Scout den. I was not a gifted athlete, but I took advantage of my early start and competed successfully for 20 years. My two brothers (who were gifted athletes, like my father) and I won the Oregon High School state championship several times. Perhaps my most memorable and formative wrestling experience occurred in 1965, when I was a sophomore in High School. Inspired by my father, who had traveled all over the world competing and coaching in international wrestling, I won a state-wide tournament that earned me a place on a Wrestling Cultural Exchange team that visited Sweden, Finland, and Poland, for 6 weeks that summer. It was my first trip out of the country, and the first airplane flight of my life was from Portland over the North pole to Stockholm. What an eye-opener for a small-town boy. We stayed in private homes, sampled the food and cultures, learned a little of each language, competed almost every day, and made life-long friends. My later decision to become a scientist was forged in no small part by that experience – I knew I wanted to be in a profession that would connect me to people all over the world.

I enrolled at Stanford, where I won All-American wrestling honors in 1971, the year I graduated from Stanford in Physics. In 1972, just after entering the PhD program in Biophysics at Stanford, I recorded my first EPR spectrum, working with Harden McConnell and Jim Hyde on the first biological saturation transfer EPR experiments. But my graduate training was interrupted when I qualified for the final Olympic Trials, which were held in Minnesota (my future home!) in the summer of 1972. Photo 2 shows me (in my wrestling costume) and my father at that time. He was extremely proud that all three of his boys made it to the finals, although none of us won a spot on the team. My excuse was a good one: the guy who won the trials and went on to the Olympics was Dan Gable, who went on to win the Gold Medal that year and to become the most famous wrestler in US history. I continued to wrestle throughout graduate school, even though McConnell did not approve for fear I would hurt my brain and no longer understand EPR theory.

Wrestling is not for everyone. It is the most physically demanding sport, requiring strength, flexibility, speed, endurance, weight control, strategy, and pain tolerance, while pitting two combatants directly against each other, with the ultimate goal of control and domination. This can be both physically and mentally punishing. A defeat in wrestling can be profoundly humiliating and discouraging. Like most wrestlers, I suffered through my share of painful injuries (knees, elbows, shoulders, back, fingers, nose). But it is precisely the difficulty ▶

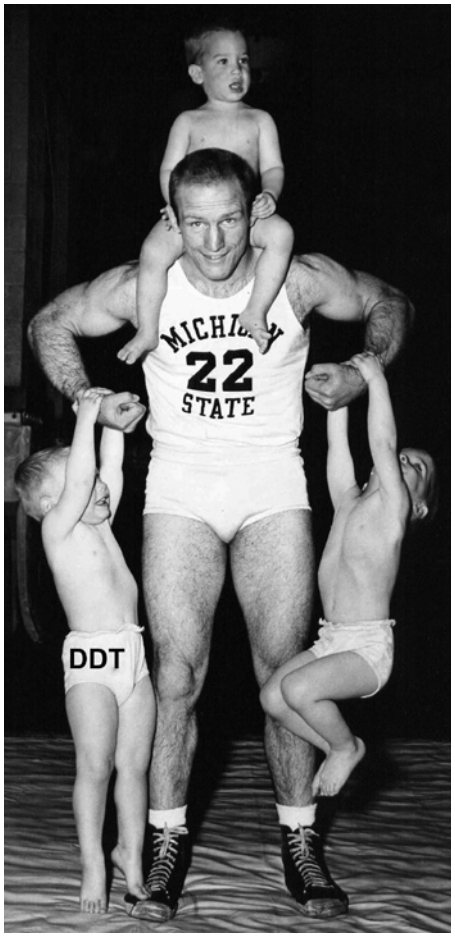


Photo 1. Dave Thomas (left) and his father and two wrestling brothers.

of this challenge along with the intencity of effort required, that makes success in wrestling so exquisite, and makes wrestlers so passionate about their sport. One of my most profound successes in wrestling was born of defeat. In 1971, in my senior year at Stanford, I was wrestling in the Pac 8 tournament. It was necessary to place in the top 3 to qualify for the national (NCAA) tournament. I received an unlucky draw. In the quarterfinals, I wrestled Larry Owings, a wrestler from the University of Washington who was famous for being the only wrestler to ever defeat Dan Gable (see above!), which he had done in the NCAA finals the year before, earning him the Outstanding Wrestler trophy. Owings was a monster, and he nearly turned me inside out. I survived the match, but I had nothing left after this physically and emotionally exhausting experience. 30 minutes later, I had to start a grueling series of consolation matches. Somehow, I found the strength to win each one of those four matches by 1 point, qualifying me for the NCAA tournament two weeks later. At that tournament, I received another unlucky draw. Again in the quarterfinals I met the defending national champion, Darrell Keller, who went on to defeat Owings (see above!) in the finals and earn the Outstanding Wrestler trophy. Once again, I was completely defeated and exhausted, and once again I had to compete in the consolation bracket with no rest. But I had faced this kind of challenge before, and my effort was rewarded with All American honors.

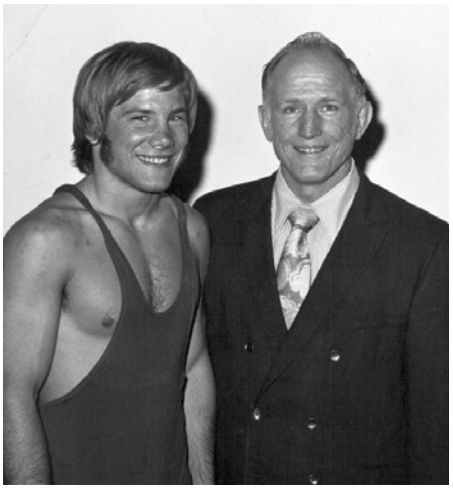


Photo 2. Dave Thomas (left) and Dale Thomas (right).

The lessons I learned that year about dedication and perseverance have been among the most important of my life.

For me, there was even more passion about wrestling that was derived from my professional environment. Wrestling is a superb combination of applied physics and physiology, and I believe that it led me naturally to research on muscle biophysics. Wrestling provided essential inspiration for me to apply EPR to understand the molecular mechanics of muscle, which has been a consistent theme in my research ever since my early work with Hyde and McConnell. In addition to the scientific benefits of this synergy, it has helped me start many conversations over the years with my wrestling friends. "What do you do?" they ask. "I do research on muscle contraction," I answer, and everybody is on the same page. In fact, one of the most satisfying experiences of my professional career was when I was invited by my father's department (Physical Education and Human Performance) to present a lecture on muscle biophysics. I showed those faculty and students of Physical Education and wrestling how EPR has played a major role in explaining the molecular basis of their craft.

I'm too old to wrestle competitively now – it's a young man's sport – but I enjoyed my role for many years as a 'counselor' in Dr. Dale's Wrestling Camp, a summer camp for young wrestlers held at my father's Double D Ranch in the coastal mountain range in Oregon. It was in this setting that I obtained much of my practical experience at teaching. Following my father's lead, our emphasis was not on winning the next match, but on developing the whole person. I discovered a profound truth about teaching that has carried through into my scientific life – I realized the depth of my passion for wrestling only when I was able to convey it to others. After my father's death in 2004, the camp closed and my wrestling coaching career ended. However, I still attend wrestling matches, and I still recall vividly the thrill of competition and the unique satisfaction that comes from complete physical and mental exertion. Now I tell my wrestling stories to my EPR students, and I hope it helps them see the rewards of personal dedication, sacrifice, and intensity. But that's another passion…

Bruker Pulse EPR
20 Years of Innovation

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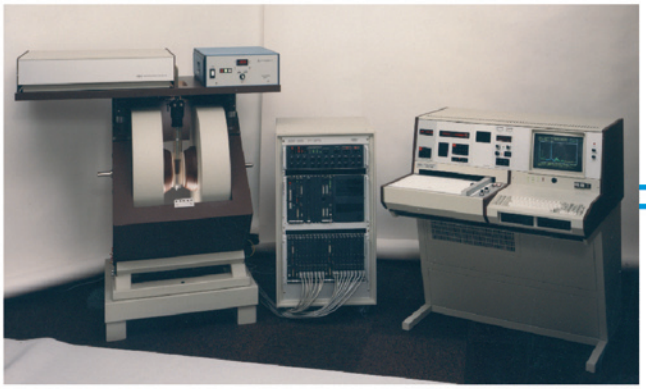

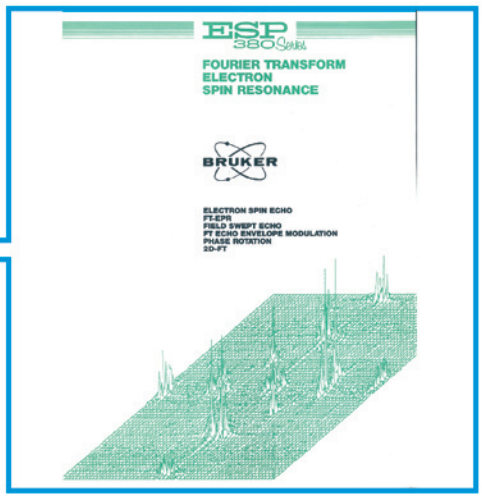

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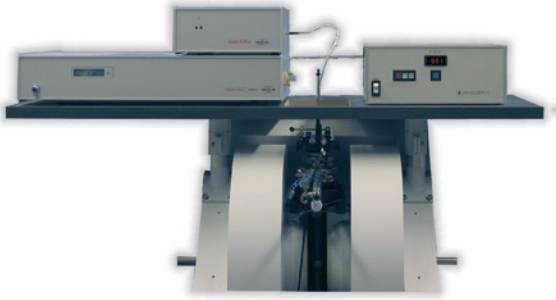
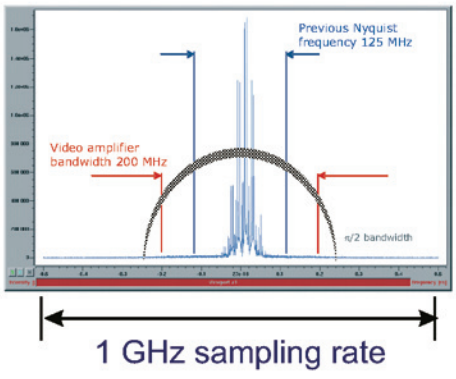
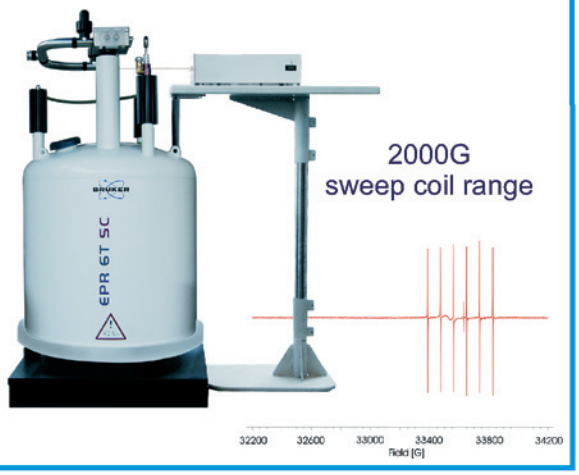
X -Band with L -, S -, Q - or W-Band



SpecJet-II:
2nd generation transient signal averager



EPR 6T SC: 2nd generation W-Band Magnet

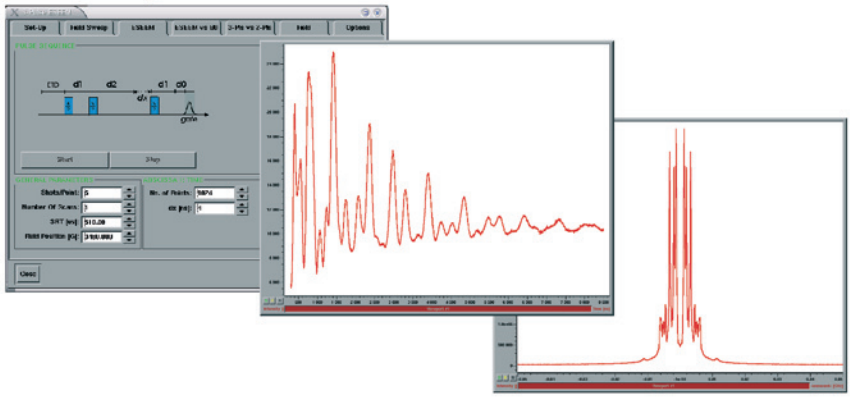


Pulse EPR
20 Years of Evolution

Method Development

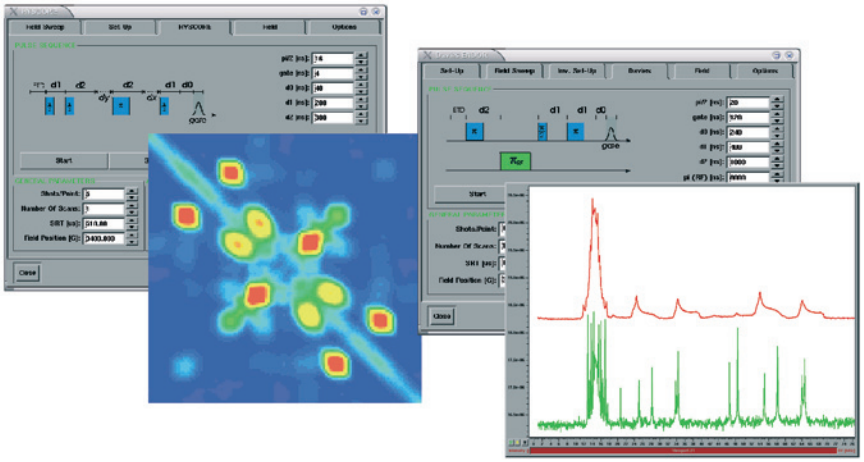
Instrument Evolution

the 80's
2- & 3-pulse ESEEM



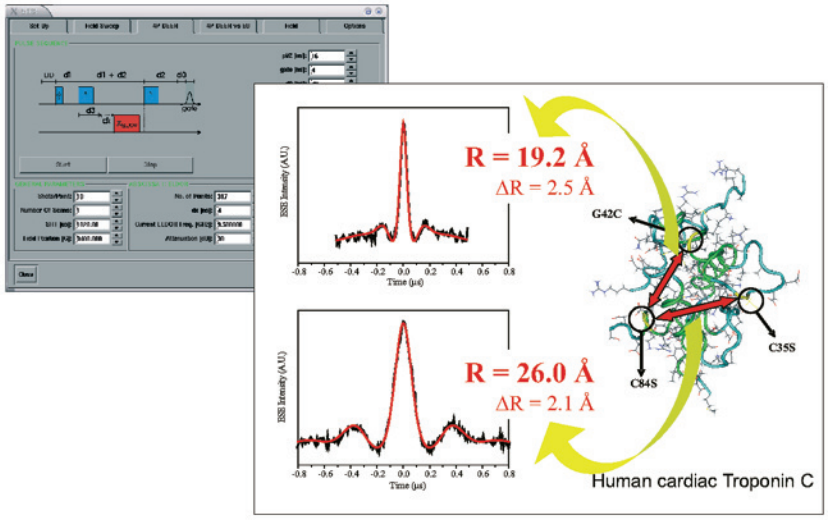
ESP 380
1st Generation
X-Band Spectrometer

the 90's
HYSCORE & ENDOR



ELEXSYS 580
2nd Generation
X-Band Spectrometer

the 00's
DEER & SR-ELDOR



ELEXSYS
3rd Generation
L-, S-, X-, Q-, and W-Band
Spectromters

ESE in Biology
Bill Mims' Reminiscences
part I

Throughout his remarkable career, Bill Mims has been a pioneer in the field of pulsed EPR on many fronts. Early on he used electron spin echoes to study fundamental magnetic resonance phenomena such as relaxation and spectral diffusion in inorganic crystals. Not content with simply subjecting the electron spins to oscillating magnetic fields, Bill developed Linear Electric Field Effect spectroscopy as well as the three-pulse ENDOR experiment that bears his name today. In the electron spin echo decay traces used to study relaxation behavior, researchers often observed a modulation pattern derived from nuclei coupled to the electron spin which complicated the extraction of parameters. Bill took this initially annoying phenomenon and put it on firm theoretical ground in two landmark publications in 1972. Then, together with Jack Peisach, he introduced the new Envelope Modulation experiment to the realm of metallobiochemistry and revolutionized the application of EPR to molecular structure determination. He has made significant and lasting contributions to all aspects of the field of pulsed EPR: basic theory, instrumentation development, spectral analysis and applications to a variety of systems. His papers are required reading for students entering the field, which is a true indication that his body of work has laid the foundation for pulsed EPR spectroscopy.

The following three articles (Parts II and III will be published in the EPR newsletter 17/2 and 17/3, respectively) are taken directly from notes made by Bill in 1985, which he passed on to Jack Peisach some 20 years later. They were initially read by a few researchers in the field, who made it clear that these historical notes would be of great interest to the EPR community as a whole. With some urging Bill reluctantly allowed them to be published. We are grateful to Bill for his incredible contributions to science and for his permission to publish a few stories on how they came to be.

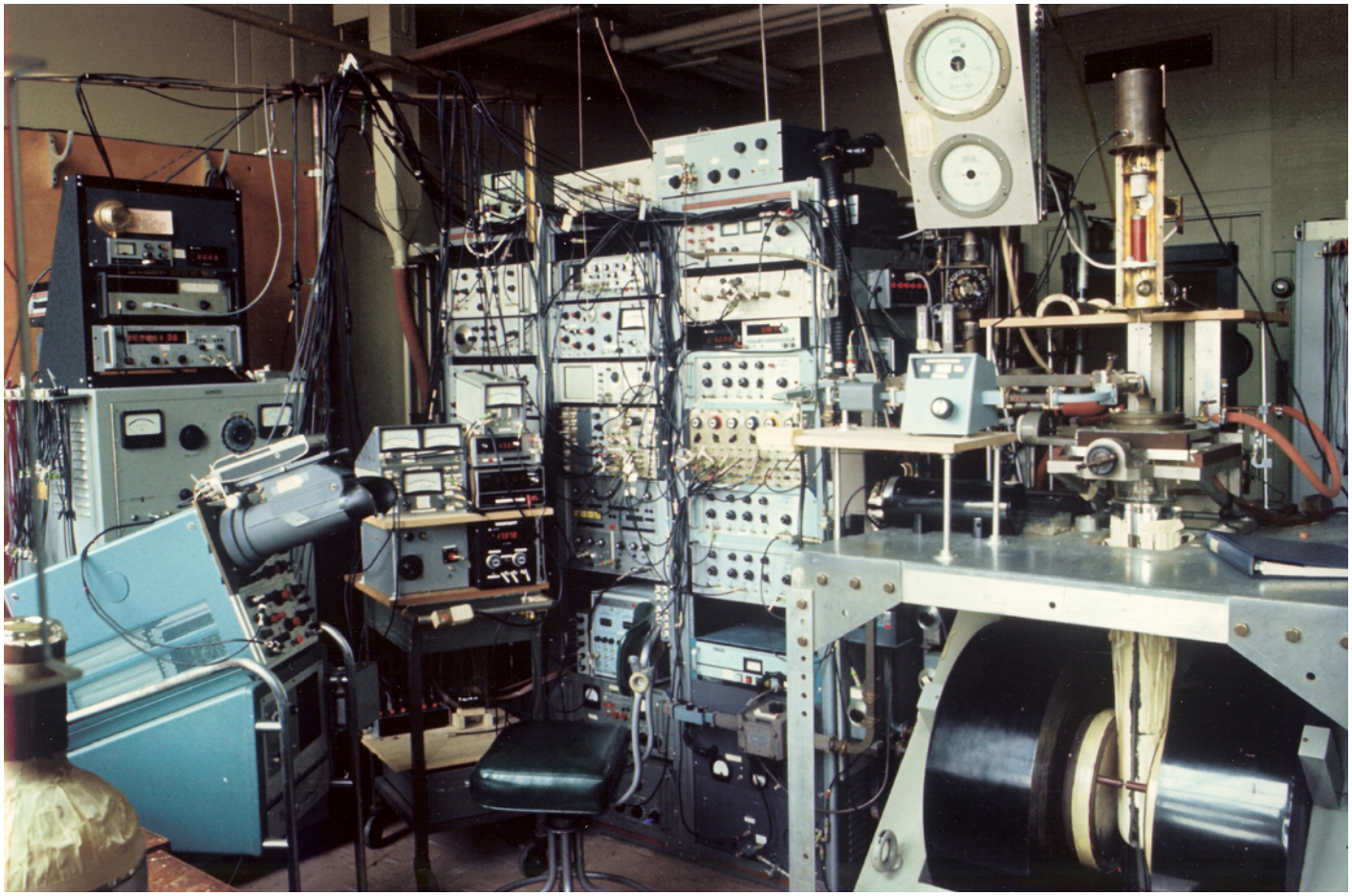
The text here is a copy of pencil notes made in August 1985 several months after my retirement while memory remained fresh. Apart from the insertion of extra commas, paragraphing, and the substitution of a few words and phrases where this seemed necessary for clarity, the text remains exactly as written until near the end, where some of the less interesting material has been truncated and the text suitably edited. It describes how the small subfield of Electron Spin Echoes in Biology grew from its first tentative beginnings in Bell Labs up to the time where similar work was being performed in half a dozen or more labs, in America and elsewhere.

These early developments were the work of two researchers, Professor Jack Peisach of the Einstein College of Medicine, and myself at Bell Labs, aided each of us by one technician. We brought entirely different scientific backgrounds and skills to the project, overlapping only to the extent that we each needed to have some understanding of the fields in which the other possessed experience. There was no duplication, but a smooth collaboration that made it possible to identify and solve the numerous problems that arose in the course of the work.

Early Plans

By the later nineteen sixties, at the end of the West Street episode, during which several of us who were members of the research staff worked in the old Bell Labs building on West Street in Manhattan, it became clear to me that the physics of electron spin echoes (ESE) and spin-lattice relaxation was done. Those parts of the subject that were amenable to tidy explanations of the kind favored by physicists had been so explained. So it was time to look elsewhere, either in physics itself or in some borderland area. One obvious course was to turn old physics into new by transposing microwave concepts into the optical range. (This was later done by R. G. Brewer at the IBM labs in San Jose.) Another interesting if less promising line was to try and use ESE techniques in order to get new kinds of information on metalloprotein samples, such as those which Jack Peisach had been bringing to the West Street lab for conventional EPR studies, working in collaboration with Bill Blumberg, another Bell Labs staff member.

This latter line of research appeared at first somewhat unpromising. Attempts to study these samples by ESE methods were disappointing enough to suggest that there might be something intrinsically different about biological samples, and my only reason for risking more time on them was the private conviction, stemming from many experiments on the 'easy' material calcium tungstate, that echo experiments could yield an order of magnitude more information than conventional EPR. The conservative approach was to improve the echo technique in ways that might make it better suited to experiments on biological materials. An obvious difficulty in the case of biological samples was the universal presence of hydrogen nuclei. The large nuclear moment of hydrogen results in large dynamic ▶



The pulsed spectrometer built by Bill Mims at Bell Labs as it appeared in 1981. A key component is the circular brass object mounted in the upper left – when all seemed lost in an experiment, the cord was pulled to play the Colonel Bogey theme in an attempt to reverse the spectroscopic fortunes.

perturbations of electron spin precession and in short phase memory times. To get a better understanding of this problem in an otherwise familiar context I made a series of studies on lanthanum magnesium double nitrate, a well known hydrated crystal, doped with various paramagnetic ions. The results showed that measurements could, with difficulty, be made, using the ESE spectrometer then available (200 ns microwave pulses), and that the hydrogen content in the material was the essential problem. Phase memory times could be approximately estimated from the g-values of the electron spin in the dopant ion.

The next stage in the experiment – deuteration of the crystals – yielded results that were puzzling. The memory times were no better, and were sometimes worse than in the protonated crystals. There were no other surprises; the ESE signals were similar, and the linear electric field effects were essentially the same as for the protonated crystals, in keeping with expectations, but the anticipated lengthening of the phase memory times (by somewhere between 6:1 and 36:1) simply did not occur. It was not until several years later that I found out that the nuclear modulation depth was three times greater for deuterium than for hydrogen, and that, by cutting down drastically on the echo amplitudes, this gave the appearance of a short phase memory. (If I had been able to read Russian I might have found this comment hidden in the text of a 1968 paper by the Novosibirsk group.)

Meanwhile it had become clear that, if the ESE method was to be of general use, and not limited to a few materials with favorable properties, a considerable improvement in the time resolution of the apparatus would have to be made. The target was an improvement by a factor of 10, i.e. by reducing the microwave pulse length to 20 ns. The considerable expense involved in making this improvement (considerable on the scale of conventional EPR spectrometer costs) was probably the reason why so few other groups had entered the field at this stage. Someone had first to risk the investment and then prove that it had been justified. Fortunately, this work was strongly supported by the lab director Rudolf Kompfner, who had invented the traveling wave tube, and who was especially interested to see this device used as both microwave transmitter and microwave receiver in the new system. Because of various disturbances in my own affairs - the move out of the West Street lab, that was being closed down, a year of absence for myself at UCLA, and the subsequent need to commit the equipment to providing a suitable project for a post doctoral at the Bell Labs Murray Hill location, – two years elapsed before what became known as ESE spectroscopy could go ahead. The primary aim was to demonstrate that problems posed by nuclear magnetic moments did not pose an unsurmountable obstacle to the wider application of these methods. Later after some attempts with doped sodium chloride and potassium chloride crystals, doped calcium fluoride was finally chosen as the material on which the initial tests would be performed. The ^{19}F nucleus has a magnetic moment almost as large as that of hydrogen, and practical difficulties might therefore be expected to be about the same as in the far wider range of hydrated materials encountered in biology and chemistry. Calcium fluoride was in addition a simple well-understood material,

crystals of high purity could be obtained, and there was a good prospect of making a series of clean, easily interpretable physical measurements, while gaining experimental expertise with the new equipment.

The Initial P-450 Experiment

Towards the end of the fluoride experiments, in early 1973, a regular collaboration with Jack Peisach was initiated in order to explore biological applications. In fact, we tried one of the more difficult experiments first – the measurement of the linear electric field effect in an iron-containing protein. From the tungstate and fluoride work I had seen that this type of experiment provided a refined structural probe of a kind not offered by conventional EPR, and I was, at the time, convinced that this technique, if it could be made to work on such samples, would be immensely valuable in the study of complex biological molecules. Only later, with more experience in the biological area, did I come to appreciate that this promise was unlikely to be fully realized because of the great difficulty of preparing single-crystal samples. That these early experiments succeeded at all was due in no small measure to the persistence of my collaborator, who insisted that we should continue, on a regular schedule, until we had gained enough experience, negative or otherwise, to make an informed judgment as to the usefulness of this experimental approach. It came as a novelty to me to find out that, in biology, qualitative information had a very real value, and that the simplicity and precision of physics was not an absolute requirement. However, I was dismayed at the very small amplitude of signals obtained with these samples. With the new high time resolution equipment this could no longer be blamed on the shortness of the phase memory times in hydrogenous media. It was clear that much of the difficulty arose from the fact that the samples were non-crystalline frozen solutions, and that echoes could only be generated by that small fraction of the electron spins whose effective *g*-values contributed to resonance in a 10 G interval. Since the overall resonance was spread over a more than 1000 G interval in the samples which we were examining, the echo signals were comparable to those one would obtain with a single crystal with a much lower concentration of paramagnetic ions. But fortunately there was also some good luck along the way. It turned out that the high values of the stepped electric field needed in the experiment (up to 100 kV/cm) could be sustained by the aqueous protein samples, once they had been cooled to helium temperatures, as required for echo generation.

The first set of electric field effect measurements on the iron-containing protein cytochrome P-450 were performed with the microwave cavity and electrode structure used in the earlier calcium fluoride series of experiments. With the same setup a new series of measurements were then started on the ferric center in oxidized cytochrome-c. This represented something of a retreat, since there were fewer scientific questions to be solved here, but it seemed necessary at the time to generate confidence in these methods, which were wholly unfamiliar to biologists, by testing them out on a protein whose structure and properties were well known.

Throughout this time I had also been trying to think of ways to overcome some of the practical difficulties encountered in these experiments, and to improve the dismal signal to noise parameters. An obvious approach was to try signal averaging, and some special circuits, suited to the conditions of the electric field effect experiment, were hastily designed and installed. Problems of a different kind lay in the mounting of the sample, which was liquid at room temperature, in the attachment of the required high voltage electrode, and in the precise determination of the sample thickness after it had been frozen. Later several attempts to redesign the sample enclosing capsule, which was mounted in the same way as the calcium fluoride crystals had been mounted, I decided to go for an entirely different design of the microwave cavity, in which the high voltage electrode would also serve as the microwave resonator, and in which the sample could be introduced at room temperature without undue difficulty. As an additional bonus this design would increase the sample filling factor by 20:1, and should therefore improve the signal to noise performance.

From the first minutes of experimentation with this new microwave cavity-electrode structure we could see that the last three-months data taking had been largely superfluous. Better results could now be obtained in a single day's work. The cytochrome-c experiments were quickly concluded, and a new and more elaborate series of measurements on heme compounds (analogues and derivatives of the heme centers found in hemoglobin and myoglobin) were initiated.

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Tips & Techniques

TenSorS in Magnetic Resonance Spectroscopy

John A. Weil

Not all members of the magnetic resonance community have the realization that the common generally angle-dependent properties (scalars g, g_n, D, A, P, …) are not obviously related to *tensors* as carefully defined by mathematicians. Thus, despite the frequent usage by some scientists of the word 'tensor', it is far from obvious that there is such a thing as (e.g.) a g tensor (Zeeman splitting for electron), a g_n tensor (Zeeman splitting for nucleus & chemical-shift tensor), or an A (hyperfine) tensor, as is stated in some of the literature. Herein, the 'ins and outs' of the concepts involved will be explored.

Consider any real 3×3 matrix

$$\mathbf{M} = \begin{matrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{matrix} , \qquad (1)$$

i.e., a set of 9 scalars (18 if the elements were allowed to be complex). The set may be merely a 'simple' array of numbers with no other mathematical properties. Usually however, other aspects are specified.[1] For our purposes, we differentiate between parameter matrices and transformation matrices (see below).

When the matrix **M** is a parameter matrix **Y** (i.e., describing some physical property of the system considered) then the sub-indices of its elements $Y_{\alpha\beta}$ (range $\alpha,\beta = 1,2,3$) may indicate action on the physical system of two different physical 'agents' (e.g., $\mathbf{E}^T\cdot\mathbf{Y}\cdot\mathbf{F}$) described using the same 3-space coordinate axis set. However, alternatively, it is legitimate and possible to describe the two agents by using two *different* sets of coordinate axes.

Often in science, one associates transformation properties under coordinate transformations with the sub-index labels of a matrix **M** = **R**. And, one can associate such behavior *separately* for each member of the index pair. Thus, the human in charge has the freedom to construct relationships between two different coordinate systems, each linked to one of the indices. Generally, **R** is real orthogonal but not symmetric.

When both indices are *linked* to the *same* coordinate system, we can (and formal mathematicians do) call **Y** a 2nd-rank tensor, providing that **Y** describes some physico-chemical property of a natural system and obeys the relation[2]

$$Y'_{ab} = (\mathbf{R}\cdot\mathbf{Y}\cdot\mathbf{R}^T)_{ab} = \Sigma_{\alpha\beta}R_{a\alpha}R_{b\beta}Y_{\alpha\beta} , \qquad (2)$$

where integers α, β, a, b all range from 1 to 3 (for instance, see [1], eq. 3.19) when the coordinate system is changed via one or more proper (or improper) rotations (**R**) of the coordinate axes. Here symbol · denotes matrix multiplication. Superscript T denotes transposition, of a matrix [or of a vector (column ↔ row)]. However, if the indices are linked to *different* coordinate systems, then **Y** is *not* a true tensor. Thus a 2nd-rank tensor is a 3×3 matrix, but a 3×3 matrix is not necessarily a 2nd-rank tensor.

The relationships between the concepts 'matrix' and 'tensor' are also discussed by Goldstein et al. [2]. The term 'tensor' (most important in our case above: the second-rank' tensor) is rigorously defined in the text book by Nye [3]. Nye carefully defines the terms 'matrix' and 'tensor', and also points out (p. 35) that all tensors can be represented by matrices, but that the converse is not true. For similar information, also see the books by Arfken & Weber [4], Brand [5], Lovett [6], Sands [7], and by Wooster [8].

It will now be useful to consider pseudo-tensors. Pseudo-vectors, alias axial vectors, (unlike polar vectors) are invariant under the spatial inversion operation on the coordinate system, which changes a cartesian set between left and right. Polar vectors change sign upon inversion. On the other hand, pseudo-scalars are numbers which change sign under such transformation, while ordinary scalars do not. A pseudo-tensor is a quantity which transforms like a true tensor under spatial rotations, but which transforms like a true tensor plus a change of sign of all its components under spatial inversion. Note the major difference between the above 3 definitions of 'pseudo'.

We shall now consider various examples of matrices **Y** as they occur in a routine spin Hamiltonian, such as is set out below. Matrices **g**, $\mathbf{g}_n$ and **A** are not necessarily symmetric (however, in practice this effect is usually ignored).

A basic reason for existence of the above-stated problem is that the parameters cited are linked to quantum-mechanical angular-momentum (spin) operators, for instance via the 'usual' spin-Hamiltonian operator

$$H_S = \beta_e\mathbf{B}^T\cdot\mathbf{g}\cdot\mathbf{S} - \beta_n\mathbf{B}^T\cdot\mathbf{g}_n\cdot\mathbf{I} + \mathbf{S}^T\cdot\mathbf{D}\cdot\mathbf{S} + \mathbf{I}^T\cdot\mathbf{P}\cdot\mathbf{I} + \mathbf{S}^T\cdot\mathbf{A}\cdot\mathbf{I} + \ldots , \qquad (3)$$

appropriate for presence of a single electron paramagnetic system (spin **S**) and one nuclear spin (**I**). Here H_S, **S** and **I** (but not applied magnetic field **B**) are operator matrices (n×n) in the n-dimensional spin space, symbols **B**, **S** and **I** are pseudo-vectors (and represented by column vectors = 3×1 matrices) in our usual 3-space (Euclid et al.), while **g**, $\mathbf{g}_n$, **D**, **P** and **A** are 3×3 matrices expressed in that 3-space.[3] Each such parameter matrix generally has its own principal axis system. We note that the **g**, $\mathbf{g}_n$ and **A** terms in Eq. (3) contain two *different* spin operators, while the **D** and **P** terms contain the same such operator twice. Hence the two indices in the matrices **D** and **P** necessarily refer to the same coordinate system.

We can call the terms shown explicitly in Eq. (3) 'quadratic' terms; other (higher-order) terms can exist [9], Sect. 6.6. The above spin Hamiltonian is used to obtain the energies (and hence also transition energies) of the spin system considered. Another, similar ▶

[1] An important consideration is whether the matrix (tensor) **Y** is a symmetric one. If so, its principal axis system is an orthogonal set, and otherwise not. In the symmetric case, the principal axis system is cartesian. Also, here, one need not consider the difference between covariant and contravariant indices [2]. With skew-symmetric tensors, the principal axes are not orthogonal. When one can restrict oneself to coordinate transformations between orthogonal-axis sets, one can limit oneself to 'cartesian' tensors [15].

[2] Valid for axial tensors and also for polar tensors (see the text). Note also that, for the sake of simplicity, we'll ignore translations of the origins of the axis sets.

[3] Also see papers by Skinner & Weil [13, 14], wherein some of the same problems are discussed in terms of polyadics. Thus the physical parameters are contained in the polyadics, with (e.g.) dyadics represented by 3×3 matrices.

spin Hamiltonian with the excitation magnetic-field amplitude vector $\mathbf{B}_\mu$ replacing **B** in Eq. (3), yields the transition relative intensities. The line positions and intensities obtained are expressed in terms of the scalar ('tensors' of 0th rank) parameters g, g_n, D, P, A, …, derived as projections from the matrices **g**, $\mathbf{g}_n$, **D**, **P** and **A** [10].

See Abragam and Bleaney's book [11] for some discussion of the situation for matrix **g**, wherein it is stated that **g** is not a true tensor. The essence here is the difference between the concepts of actual spins and fictitious spins.

One question to be settled is how the formal definition of 'tensor' involves the quality of the vectors projecting onto **Y**, i.e., how are products of type $\mathbf{E}^T\cdot\mathbf{Y}\cdot\mathbf{F}$ affected by whether vectors **E** and **F** are axial or polar [12]. The latter authors, Pake and Estle, make the statement that (e.g.) **g** is not a true tensor due to this characteristic. Our thought is that both axial and polar tensors are tensors as defined by mathematicians. Then too, the question arises: if **Y** is a tensor, how does one decide in practice whether it is an axial tensor or a pseudo-tensor?

It appears that the 3-space basis associated with each spin vector operator is 'arbitrary'. Thus operator **S** (and/or **I**) need not necessarily be taken as quantized along some obvious physical direction, such as that of an applied magnetic field **B**. In other words, spin operators **S** and **I** need *not be expressed in the same space*, i.e., to be quantized along the same spatial directions (i.e., the spin projection quantum numbers may be measured along different selected directions in our 3-space). The most general case, which occurs when the two quantization axes are not aligned, prevents the parameter matrices from being tensors.

One can explore what functions of each parameter matrix are actually obtainable by scientists using the above spin hamiltonian, via the measurable line positions and relative line intensities of magnetic-resonance spectra; see publications by Skinner and Weil [13, 14] for some aspects of this. The question as to which parameter matrices occurring in Eq. (3) are directly available from experimental data is far from trivial [10, WB07]; matrices **g**, $\mathbf{g}_n$ and **A** are not, while their squares (see below) are.

The 3×3 matrices $\mathbf{g}^T\cdot\mathbf{g}$, $\mathbf{g}\cdot\mathbf{g}^T$, $\mathbf{g}_n^T\cdot\mathbf{g}_n$, $\mathbf{g}_n\cdot\mathbf{g}_n^T$, $\mathbf{A}^T\cdot\mathbf{A}$, $\mathbf{A}\cdot\mathbf{A}^T$, **D** and **P** are all true 2nd-rank tensors, whereas **g**, $\mathbf{g}_n$ and **A** are not necessarily so (note [9], Sect. 4.4). Note that the task of deconvoluting (say) $\mathbf{g}^T\cdot\mathbf{g}$ to arrive at **g** is a vexing one; for instance, the 'sign' of **g** is not readily available (i.e., all of the 9 elements of **g** can be multiplied by −1 with no change to $\mathbf{g}^T\cdot\mathbf{g}$). However, the sign is available from det(**g**), which is measurable, if **g** is not singular (see [9], Sect. 4) [13, 14]. Attaining matrix $\mathbf{A}^T\cdot\mathbf{A}$ or $\mathbf{A}\cdot\mathbf{A}^T$ has its own problems (see [9], Sect. 6.7).

The question of whether matrix **g** can be singular, symmetric, or even complex must be left for another discussion. Similarly, the relationship between the matrices occurring in quadratic terms in H_S of the form $\mathbf{E}^T\cdot\mathbf{Y}\cdot\mathbf{F}$ and the 'opposite' form $\mathbf{E}\cdot\mathbf{Y}'\cdot\mathbf{F}^T$, when $\mathbf{E}\neq\mathbf{F}$, also deserves some discussion.

Much of the above is predicated on the major question, still to be completely and formally settled, as to whether, in quantum mechanics, specification of the quantization axis $\mathbf{Z}_1$ for one spin leaves the quantization axes for all other spins in the system arbitrary, rather than compelling all of these to be identical to $\mathbf{Z}_1$.

The author would be most pleased to learn from readers what they know about this point, and about any other aspects of the above composition.

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Blank A., Dunnam C.R., Borbat P.P., Freed J.H.: Appl. Phys. Lett. **85**, 5430–5432 (2004), www.acert.cornell.edu/PDFs/ApplPhysLett85_5430.pdf.

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Costa-Filho A.J., Crepeau R.H., Borbat P.P., Ge M., Freed J.H.: Biophys. J. **84**, 3364–3378 (2003), www.acert.cornell.edu/PDFs/BiophysJ84_3364.pdf.

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Interested qualified candidates should direct their inquires to acert@cornell.edu.

Applicants should provide a cover letter and most recent CV. Two or three letters of recommendation are also required.

Additional information about the ACERT may be found at www.acert.cornell.edu.

Director, Electron Magnetic Resonance Program

The National High Magnetic Field Laboratory in Tallahassee, FL is seeking a senior researcher in electron resonance to lead the existing EMR program. The program currently comprises four faculty-level in-house scientists who develop high field instrumentation, assist the external users, and develop their own research interests. In addition to the in-house research and outside collaborations, there is strong interaction with the EPR laboratories at Florida State University (FSU) and the University of Florida (UF) in the areas of structural biology, chemistry, physics, material science and computation. The EMR program features unique high-frequency spectrometers (up to 800 GHz) and access to uniquely high magnetic fields (up to 45 T). Research focus includes nano-scale magnets, metallo-proteins, and instrument and technology development for high-frequency, time-domain EMR. Other opportunities include the use of a unique THz-Infrared light source currently under design for installation at the NHMFL in the five- to ten-year timeframe.

Minimum qualifications include a PhD in Physics, Chemistry, Biology or related. The successful candidate has a track record of outstanding scientific scholarship, and is expected to define and develop a multidisciplinary long-term vision for the program. Senior scientists with a strong international reputation, strong publication and grantsmanship records are encouraged to apply. Particular research interests in one or more of the following areas is preferred but not required: molecular magnets and other nano-scale magnetic material and/or ▶

metallo-protein structure and function. The appointment will be either at the Scholar Scientist level (non-tenure track) in the NHMFL or a Professorial position in an appropriate academic department at FSU.

To apply, please send your curriculum vitae, cover letter describing your experience, and names and contact information of three references to Professor Peter Fajer, Chair, EMR Director Search Committee, National High Magnetic Field Laboratory, Florida State University, 1800 E. Paul Dirac Drive, Tallahassee, FL 32310-2740, 850-645-1337, fax 850-644-1366; or e-mail fajer@magnet.fsu.edu. The selection will start on April 15 and will continue until position is filled. An Equal Opportunity/Access/Affirmative Action Employer.

Faculty position for an EPR scientist

The Division of Cardiovascular Medicine, Brigham and Women's Hospital, is seeking a research scientist with experience in electron paramagnetic resonance to fill a faculty position. The candidate should hold a PhD and/or MD degree with at least 2-3 years postdoctoral research experience. The successful candidate is expected to establish a research program in collaboration with faculty members interested in the role of oxygen and reactive oxygen species in cardiovascular physiology and disease using EPR technology. This position offers an attractive start-up package including appropriate instrument support.

Interested applicants should submit a C.V., a brief statement of research interests, and the names of three references to: Faculty Search (attn: Linda Johnson), Brigham and Women's Hospital, 221 Longwood Avenue, Room 247, Boston, MA 02115 or ljohnson@rics.bwh.harvard.edu (subject: EPR faculty search).

Brigham and Women's Hospital is an equal opportunity employer. Women and minority candidates are particularly encouraged to apply.

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