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Shimon Vega in the eyes of his students and postdocs

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ABSTRACT

Professor Shimon Vega (1943–2021) of the Weizmann Institute of Science passed away on the 16th of November. Shimon Vega established theoretical frameworks to develop and explain solid-state nuclear magnetic resonance (NMR) and dynamic nuclear polarization (DNP) techniques and methodologies. His departure left a profound mark on his many students, postdocs, and colleagues. Shortly after his passing, we all assembled spontaneously for an international online meeting to share our reflections and memories of our experiences in Shimon's lab and how they affected us deeply during that period of time - and throughout our scientific careers. These thoughts and feelings were put here into writing.

Introduction

Professor Shimon Vega (1943–2021) of the Weizmann Institute of Science passed away on the 16th of November. Shimon Vega established theoretical frameworks to develop and explain solid-state nuclear magnetic resonance (NMR) and dynamic nuclear polarization (DNP) techniques and methodologies. His departure left a profound mark on his many students, postdocs, and colleagues. Shortly after his passing, we all assembled spontaneously for an international online meeting to share our reflections and memories of our experiences in Shimon's lab and how they affected us deeply during that period of time and throughout our scientific careers. These thoughts and feelings were put here into writing.

Shimon Vega, April 3rd, 2012, Weizmann Institute (FMV)

1. Amir Goldbourt

When I was a PhD student with Shimon, Cohen-Tannoudji visited the Weizmann Institute. Perhaps his most memorable advice was how to pick your supervisor. He said – "find a person that you like and the science will be great." I thought how lucky I was to choose the right supervisor. I was learning from an amazing scientist but, moreover, a unique human being that always gave you the feeling that you are the most important person in his life at that moment and those that follow. The years 1996–2003 will always be engraved in my memory.

I joined Shimon's lab as I wanted to see in my own eyes how quantum mechanics comes to life in experiments, and magnetic resonance was the right choice for that. Shimon made quantum mechanics real and beautiful. For that reason, although Shimon suggested that I work on ^{2}H NMR (which I did at the beginning), I was asking for more energy levels. Thus, my PhD studies focused on half-integer quadrupolar nuclei. From Shimon's perspective that only meant that the math is more fun, because he could now diagonalize 4×4 and 6×6 matrices, and he could do it with ease by scratching transformation operators on the blackboard. But Shimon would make you do it yourself with his endless patience.

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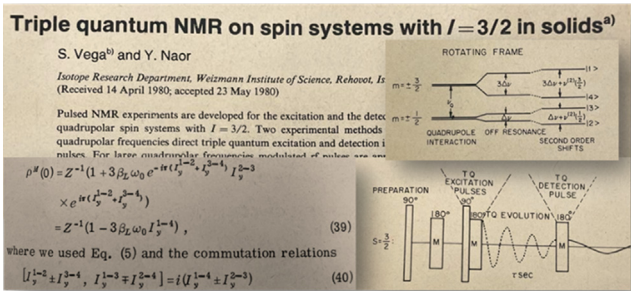
You would stand in his famous room at the end of the corridor, stand by near the blackboard, and try with all your effort to diagonalize Hamiltonians. While you are mixing up Hamiltonians with density matrices, Shimon would work on his computer and occasionally throw insightful remarks, and you would realize, that while working on his own affairs, he would still be one-hundred percent focused on your endless struggle and lead you to the correct solution. The greatness of Shimon as a PhD mentor was his ability to make you learn in a gentle and elegant way by guiding you without explicitly solving anything directly. Somehow, he would cause your mind to arrive at the correct answers.

Shimon wrote many seminal papers when I was still at elementary school, many of them on multiple-quantum NMR using fictitious spin operators. The most influential paper that goes with me everywhere (I still have the yellowish hard-copy, as authors used to get them by mail from the journal) was on triple-quantum excitation of quadrupolar nuclei [1]. I still think and feel fictitious spin-half operators, and use these tools to understand problems we encounter in our lab. I feel obliged and enthusiastic to always pursue better ways to perform quadrupolar NMR spectroscopy.


Triple quantum NMR on spin systems with $I=3/2$ in solids[a)]

S. Vega[b)] and Y. Naor

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(Received 14 April 1980; accepted 23 May 1980)

Pulsed NMR experiments are developed for the excitation and the detec quadrupolar spin systems with $I=3/2$. Two experimental methods quadrupolar frequencies direct triple quantum excitation and detection i pulses. For large quadrupolar frequencies modulated rf pulses are ap

ROTATING FRAME

QUADRUPOLE INTERACTION OFF RESONANCE SECOND ORDER SHIFTS

$$\rho^{II}(0)=Z^{-1}(1+3\beta_L\omega_0 e^{-i\pi(I_y^{1-2}+I_y^{3-4})}I_y^{3-3}$$
$$\times e^{i\pi(I_y^{1-2}+I_y^{3-4})})$$
$$=Z^{-1}(1-3\beta_L\omega_0 I_y^{1-4}), \quad (39)$$

where we used Eq. (5) and the commutation relations

$$[I_y^{1-2}\pm I_y^{3-4},\ I_y^{1-3}\mp I_y^{2-4}]=i(I_y^{1-4}\pm I_y^{2-3}) \quad (40)$$

PREPARATION TQ EXCITATION PULSES TQ DETECTION PULSE TQ EVOLUTION

90° 180° 90° 180° 180°

M M M

$S=\frac{3}{2}$

τsec

I try to take from Shimon the patience, the quest for every detail, the devotion to scientific truth and integrity, and the devotion to be there for any eager student, be it your own, or of others.

Like all great artists, Shimon's scientific song and spin art will always be with us.

2. Gil Goobes

As an undergraduate student, I had a sense that nuclear magnetic resonance is an exciting field, and probably what I will want to carry out my research on. Professor Gil Navon taught a course on magnetic resonance spectroscopy at that time and was running in parallel a graduate level course on the subject – which I, naturally, joined. Before moving to the Weizmann Institute for my graduate degrees, determined to continue with NMR, I asked the teaching assistant in the graduate course, Itamar Ronen, now Professor at the Leiden University Medical center, "who should be contacted in case I am interested in NMR theory", and his immediate response was "Shimon Vega!".

So, this has paved the way to carrying out both my MSc and PhD research with Shimon and turned out to be a judicious and gratifying experience. One aspect of working with Shimon on NMR problem solving is the perpetual test of the depth of dive into the theory that one was willing and capable of taking. You can imagine climbing a winding road to a high snowy peak with a cheerful clear-eyed guide always showing up in front of you, restless, at each curve and turn, never tired and always leaping forward two steps ahead, effortlessly. Mind you, you still had to climb up yourself, whether it was writing down the correction terms for finite-pulse XY-8 REDOR using Floquet theory or working out the analytical expressions for matrix diagonalization of homonuclear-coupled spin Hamiltonians.

One quality of Shimon, which may not strike immediately as typical of him, is his openness to new ideas and initiatives. We were allowed the time to program a Matlab code for the REDOR transform (which was already proposed by Karl Mueller at the time) and amused ourselves with possible core functions suitable for the other anisotropic interactions. We discussed ways of polarization enhancement and delved into fundamental reasons why an equivalent of stimulated emission population inversion in a MASER in the microwave region was not possible in the radiofrequency region for NMR. However, large out-of-course excursions were gently and cleverly discouraged as Shimon was too knowledgeable to allow a complete waste of time. One of the projects, in which I felt that Shimon was caught slightly surprised with an unanticipated result, was flipping individual proton lines while applying a phase modulated Lee Goldberg (PMLG) decoupling field, which we were running together with Elena Vinogradov. We tested the crystalline hydrate of histidine with its 10-proton spin system and were trying to record the magnetization transfer between protons after such DANTE-PMLG flip, only to discover that the protons would diffuse fast! too fast when the strengths of all contributing interactions were accounted for. It dawned on us then, that the sample we used was uniformly ^{13}C labeled and that the homonuclear carbon–carbon couplings would serve as a spin bath that would cause the extra leakage of spin magnetization through the non-negligible ^{1}H–^{13}C couplings. By adding CW decoupling on the ^{13}C channel through the sequence and verifying with a natural abundance histidine sample, we could confirm that this was the reason for the faster spin diffusion.

Shimon, it is the outstanding combination of your true caring mentorship and a sweeping endeavor of solving fundamental research challenges that has made the experience of spending time under your tutorship unforgettable, thank you.

3. Yonatan Hovav

I have been a student of Prof. Shimon Vega during my masters and PhD, as well as during a short postdoctoral period, with most of our period together devoted to the study of static solid state DNP. There are many praises to give Shimon as a teacher, a mentor, a scientist, and a person. Below are some glimpses into who he was to me, and I believe to his other students and co-workers as well.

I joined Shimon's Group after taking his NMR primer. Something in his enthusiasm and friendliness drew me to him. I did not have a quantum mechanics background, but was fascinated by it, and hoped Shimon would help me understand it better. To join the lab, you had to go through Shimon's fire test (I believe most, if not all, of his students passed it): "Why would you come to my lab?" he would ask, "you will need to work much harder to get the same results as in other labs". And he was right – my MSc period left me confused and with little results, at least in my mind, and yet I stayed for a PhD. It was there that all the hours spent with Shimon and his students sank in, and suddenly things made sense. I ended up spending most of my time writing and playing with quantum mechanics simulations, trying to understand the basic mechanisms of DNP.

Shimon would often say that our task in science is to transfer the knowledge from one generation to the next – starting from the giants of old and building the generation to come – and in his knowledgeable and patient way he acted on it. His door was always open to us, and we could come and ask any question. The main obstacle was finding a time where there wasn't another student in the room already, being one of his own students or not. Going into his office with a question, he would often take me back several steps to the basics, making sure I built a solid foundation in his patient way. I would then solve my question with him on the

board or at the office armed with the new understanding he gave me. He had a way of simplifying the physics – one day he took me on a *gedanken* bus ride to explain perturbation theory. But as time went on, we talked more and more in matrices and Hamiltonians, creating a Vega group shorthand DNP convention. When a hard question came, we would often work on it in parallel.

Shimon would take the research to heart, as well as his student's wellbeing. He would come to see how an experiment was going (spinning on the lab chair in his energetic way), coming to the student office to hear the latest experiment or simulation results, or calling you to his office and saying he didn't sleep at night thinking about the problem at hand. He would help out when needed, learn about what we discovered, and give direction in his gentle way: "if I were you, I would do this and that next" he would say. His reactions were often an inverse reflection of my own feelings: when I was excited about some new result, he would cool me down, talking about possible problems or the next steps; and when I was down – he would try to pick me up, pointing to past successes.

Shimon would always have something good to say about everyone. If he disagreed with the theory, he would point out to the experiment, and while he worried that a competitor would publish something before us – it always felt we belonged to the same group. While he believed in his way of thought – he tried to connect it to that of others. Before anything else, he would view you as a person, and as such would treat you in his friendly and polite way.

I feel fortunate, thankful, and privileged to have had Shimon as my Professor, and to have taken part in his group.

4. Ilia Kaminker

As perhaps all the others who have passed through Shimon's research group, I share the same experience of having to convince him to take me in. I spent six years, during my PhD with Daniella Goldfarb, sitting in the student room two doors from Shimon's office. By the time I was looking for a postdoctoral position, we knew each other. I took Shimon's NMR primer, he helped us with theory on one of my papers with Daniella, and I heard him present many times in various magnetic resonance conferences. Still, when I asked him if I could join his group, he tried, as was his custom, to talk me out of it. Fortunately, I was persistent enough and had the honor and privilege to work with Shimon for two years (2012–2014).

During that time, we worked closely with Shimon's PhD students Daphna Shimon and Yonatan Hovav, with constant support from Akiva Feintuch. When I joined the group, the three of us were working on separate projects, all having to do with understanding of DNP. Somehow, after a few months, all the projects had merged, and we realized that we are actually all working together on different aspects of one bigger problem. The combined effort during the remaining year and a half remains a unique scientific experience with the three of us under constant guidance from Shimon tackling, revealing and slowly understanding a complicated phenomenon.

Another profound influence of Shimon on me was the realization that there are different levels of understanding. All of us sometimes say to ourselves "now I understand it". Shimon had very strict requirements as to what "understanding" means. Understanding for him had to do with rigorous derivation; it had to be firmly based on the very basics of magnetic resonance and quantum mechanics. He did not believe in hand waving arguments – they never convinced him. It took me quite some time to adapt myself to Shimon's requirement of "understanding" and I am very grateful to him for this. It has undoubtedly made me a better scientist.

I greatly miss Shimon. After returning to Israel, I had many ideas that I was hoping to discuss with him. I wanted to invite him to see my lab – something that, now, will never happen. Rest in peace Shimon.

5. Vladimir Ladizhansky

I joined Shimon's group as an MSc student in 1993 on the advice of Professor Yehiam Prior, and had the privilege of spending the next six years in his lab and continuing to learn from him for much longer. My MSc and PhD theses were at the interface of chemistry and physics, focusing on the analysis of II-VI diluted magnetic semiconductors and semiconductor nanoparticles. As Shimon's main interest was in the fundamentals of NMR spectroscopy, most other graduate students and postdocs in the lab worked on various spectroscopic problems (e.g., RFDR, NMR of quadrupolar nuclei, proton spectroscopy). Early in my PhD, I became somewhat dissatisfied with my "outcast" status and asked Shimon to involve me in the spectroscopy projects. At the time, he was working on the theory of cross polarization (CP) and offered me the opportunity to join these efforts. My first assignment was to read and understand an article that Shimon had just published along with another PhD student, David Marks, in which they established a unified view of static and magic-angle spinning CP experiments [2]. The CP paper was one of my first encounters with complex NMR spectroscopy, and it served as an entry to my scientific career. I struggled with that paper back then (and still do now!) as it is quite mathematically intense, but after numerous hours of discussions, working through our disagreements together, and getting through the equations with his guidance, a consistent picture of one of the most important solid-state NMR experiments began to emerge. The CP paper shaped my understanding of dipolar recoupling experiments, and specifically those that involve strongly coupled systems.

Shimon had an amazingly clear and at the same time constantly evolving picture of magnetic resonance, and the ability to bring physics to life. His door was always open to students, and interacting with them and mentoring them were among his greatest joys. He valued our opinions and ideas even if they were nonsensical. In many ways, his influence, which was not limited just to science, had a profound impact on my life and future career. We have lost a true scientist and scholar. He will be missed dearly.

6. Michal Leskes

I got to join Shimon's group pretty randomly. I was a Chemistry undergraduate in my second year at Tel Aviv University, looking for something to do in the summer. I came across the summer program at Weizmann and thought I'd try. I quickly realized I had no idea how to choose a lab for the summer and going through the webpages of researchers at Weizmann didn't help at all, since nothing made sense. I knew I liked spectroscopy, but beyond that I decided to choose based on who was smiling in their photo – and that is how I got to Shimon Vega's group. This was probably the best career move I made... joining Shimon's group for that summer completely determined what kind of research I would do in the next few years and what kind of scientist I aspire to be.

Only in retrospect I can appreciate the dedication of Shimon. I was only a second-year undergraduate student, yet Shimon spent a few hours every day with me, teaching me the basics of NMR in solids. We would talk during the day, and he would give me questions to think about and get back to him for the next day. Taking the train from Tel Aviv to Rehovot and back every day gave me time to process these lessons. After a month Shimon said I was ready to run the first NMR experiment of ^{1}H-^{29}Si CP on meso-

porous silica (of course with guidance from Shifi Kababya). By the end of the summer, I was running variable temperature ^{13}C-{^{17}O} REAPDOR experiments, that in addition to useful dephasing curves, also caused a mini flood in the NMR room. This was a great summer and I summarized it in a poem to Shimon – 'A fun summer it's been, with magnetic resonance and O seventeen. But after all of the time you've put in, I still don't know what is spin!'

Without saying

I really did not fully appreciate this period in real time, but when I came back to Weizmann as a graduate student, I realized what a unique person and teacher Shimon was and chose to join his group for my PhD. With Shimon, and a yearly visit from Madhu, we were working on homonuclear and heteronuclear decoupling using Floquet theory to understand our results. Life was a constant debate between theory and experiment and a feeling of uncertainty and confusion. But what kept me going and kept it all fun was a kind of safety net I felt Shimon provided – I felt that Shimon had it all figured out. That in fact he had this master plan of what we were doing, and perhaps we're missing a minus sign here or factor of two there, but overall, he already knows what we will get because he solved it all late at night. I was never alone, any doubt or panic about some basic or complex concept that suddenly did not make any sense could be resolved after talking to Shimon (or after an email from him written at 4 am!). It was also great fun to argue with him about results and to be joyful together when theory perfectly matched the experiment.

Towards the end of my PhD, during my postdoc and then after joining the Weizmann Institute as faculty, I learned that Shimon was also the kindest, most patient listener. It never mattered what he was in the middle of or how stressed he was, he was always happy to take a break and talk about whatever was on my mind, be it the next scientific or personal challenge. It was such a privilege to have my office two floors above his and my NMR lab two floors below his office, making it my first stop coming up from the lab whenever we got a new scientific success or failure. It will take me some time before I don't pause on the second floor of the Perlman building. Shimon, I miss you. Thank you for all that I know and all that I don't know... and now have no one to ask.

7. Frederic Mentink-Vigier

"If you join us, then what will you do after your post-doc?" Shimon started my interview with this question. To be honest, I think the question made me join Daniella Goldfarb and Shimon Vega back in 2012. The question revealed how much he cared about the people he worked with, and this is probably the reason why, up to his illness, we have remained close.

The two years I spent at the Weizmann were very stimulating. From the very first days I was exposed to the group discussions about Liouville space, relaxation, and DNP. I was fascinated by the discussions between Akiva Feintuch, Yonatan Hovav, and Shimon but barely understood them.

Shimon's office door was always open, and we could come in anytime to bring up a question or discuss the experimental results. Shimon was a fantastic teacher for whom no question is stupid. Instead, he would not only explain in detail, but would reformulate until we really understood. The open door-policy had additional perks. During the discussion someone would come in and contribute or bring another question, expanding the scope of my initial visit.

As a postdoc, Shimon and Akiva gave me the MAS-DNP project due to my coding skills but I barely understood the theory when I started it (of course, Shimon made me familiar with it). One day, I wanted to check the cross-effect simulations and ran them in absence of microwave irradiation. The result was "weird": the nuclear polarization at steady state deviated from thermal equilibrium. I did not believe it and was sure that something was wrong with the code. Shimon had a different stance and we spent four days discussing and running simulations until we understood it. The effect was real. Shimon's attitude taught me to welcome any result that would change my view of the problem.

After two years at the Weizmann Institute, the MAS-DNP simulations officially became my project, one that I still work on. I was afraid I would lose contact with him and felt rejoice when my (French) phone plan included unlimited calls to Israel: I could continue talking with Shimon while riding my bike in the morning.

We officially continued to work together until 2017 and we last were in touch for science on a daily basis during spring 2020, when I was deriving the "Landau/Zener" cross-effect evolution operator for strongly coupled electron spins.

Shimon was always modest in his presentations and clearly was driven by the genuine interest in "understanding" any experimental observations. However, I would dare say that for him, personal relations were the most important aspect in his life. I witnessed it firsthand in his lifelong friendship with Daniella Goldfarb, Lucio Frydman, Zeev Luz and many others. As one may expect, after nine years, our relationship expanded well beyond the professional sphere. We would always begin our discussions with "How is life treating you?" or "How are the kids?" We last met at Euromar 2019 and it's hard to express how much I'll be missing him. Shimon has done his best to promote my work and help me integrate in the NMR community. He made me meet people and talk at conferences, and in that sense, he went beyond the question he asked during my interview: he helped me build my career.

He was conscious of the role of mentor, and I owe Shimon so many things that I hope the reader can measure the respect I and others have for him.

8. Madhu PK

Shimon Vega was an exceptionally kind and compassionate person and a scientist *par excellence*. My own association with Shimon as a post-doctoral fellow was from November 9, 1997, till May 9, 1999. However, our collaboration continued strongly with our joint last paper on heteronuclear spin decoupling that came out in 2017. We had very regular discussions on NMR and related science, life in general, a bit on politics, culture, and history all along till March 10, 2021, before he was admitted to a hospital. Our last discussion was on the possibilities of locking half-integer quadrupole spins, one of his favorite topics which he shared with his brother Lex. In our conversations in the second week of March 2021, Shimon also shared his pain in losing Kostya Ivanov (who succumbed to Covid-19 on March 5, 2021), a common friend and colleague of both of us.

Shimon, noted for some of the most insightful research in the area of magnetic resonance, both electron and nuclear magnetic

resonance, has influenced professionally and to some extent personally the lives of many of us who have come in contact with him. This could be in the form of graduate students, postdoctoral fellows, colleagues, course students, or listeners to one of his great talks packed with science, wit, and active involvement. His enthusiasm has been often contagious and his understanding deep enough to compel chairmen of his talk sessions to give him enough time after regular sessions to explain to the particular conference audience nuances of his theoretical ideas. These were always done with a deep flair to packed audiences. Shimon was indeed one of those rare combinations of openness to new ideas with deep-rooted knowledge on sound, pen-and-paper principles, rather than pursuing transient fashions. He belonged to that genre with a great willingness to share his knowledge with others and was a restless researcher ready to question the so-called established paradigms. His inquisitiveness had always motivated his colleagues, taking the respective research to even higher levels. Of the many contributions Shimon had made, some to highlight are in the magic-angle spinning experiments in solid-state NMR, breaking the barrier into understanding quadrupole spins, introducing Floquet theory to understanding and developing various experiments and improving resolution and sensitivity of solid-state NMR experiments, and in the last few years providing insights into the important field of DNP in NMR.

Shimon had fun doing science and was never shy of sharing his ideas and thoughts at any stage of a concept, whether published or not. For him, understanding an idea was important and the only key issue. The rest were all details for the sake of others. He was a great, active, and patient listener who put all at ease and treated others with a child-like innocence and unbridled laughter. I remember various conferences, including the Indian Magnetic Resonance Society meetings for which he came a few times, schools and workshops, and other gatherings where his infectious enthusiasm would be influencing positively the students and others and even the on-lookers. He did not know that he was a rock star, but he was indeed one in the field of NMR and in science.

The NMR community and I will definitely miss Shimon. It was indeed a privilege to have worked with him, known him a bit, and travelled and interacted with him. The dimensions of the matrices he worked with are most often boundless, and his memories with us also will remain so. *Toda Raba Shimon.*

9. Silvia Pizzanelli

I joined Shimon's lab in 2002–2003 as a postdoc with a fellowship funded by the Center of Excellence on "the origin of ordering and functionality in *meso*-structured hybrid materials" of the Israel Science Foundation and the Italian National Research Council. During my PhD in Chemistry at Pisa University under the supervision of Carlo Alberto Veracini I had studied liquid crystals using ^{2}H NMR and often had come across papers by Zeev Luz and Shimon Vega. As I wished to further specialize in solid state NMR, my obvious choice was Shimon's lab. I simply wrote him an e-mail, and he simply answered inviting me to the Weizmann Institute for a first meeting.

My project dealt with the adsorption–desorption kinetics of tetra-alanine at the surface of the pores of an MCM-41 mesoporous material. I spent the first months in the preparation of the sample. Since an aqueous solution of the peptide was to be inserted in the pores of MCM-41, I could not use the capillary condensation method, usually employed for the insertion of pure liquids. Therefore, I just added MCM-41 to the solution, but this method was fraught with potential problems, like incomplete filling, location of the solution in the extra-porous space, or instability of the MCM-41 structure. In this process, Shimon was a continuous source of critical questions and pertinent suggestions, constantly challenging the interpretation of a phenomenon through the experimental evidence. But Shimon was also a man of great humanity. When Saddam Hussein was captured during the second Gulf War, I have a vivid memory of his sense of discomfort as he could not rejoice over the misfortune of any person. Sometimes he shared with me his genuine interest in the people around us, referring either to science or to human relationships. In these small talks, he was sharp and direct, and my personal views were usually in consonance with his, which created a positive and friendly atmosphere. His humbleness still echoes in my mind in the words "there is a whole world out there" that he used to say when he came across some robust and comprehensive study of a subject he had only marginally touched.

After 2003 I chose to go back to Italy and life brought me far from the adsorption project started with Shimon. On the contrary, he went on for another ten years investigating different peptides and porous materials. Today my only regret is that I did not continue collaborating with him, although he gave me the chance to do it by giving me samples and a program for simulating MAS spectra in the presence of a two-site motion.

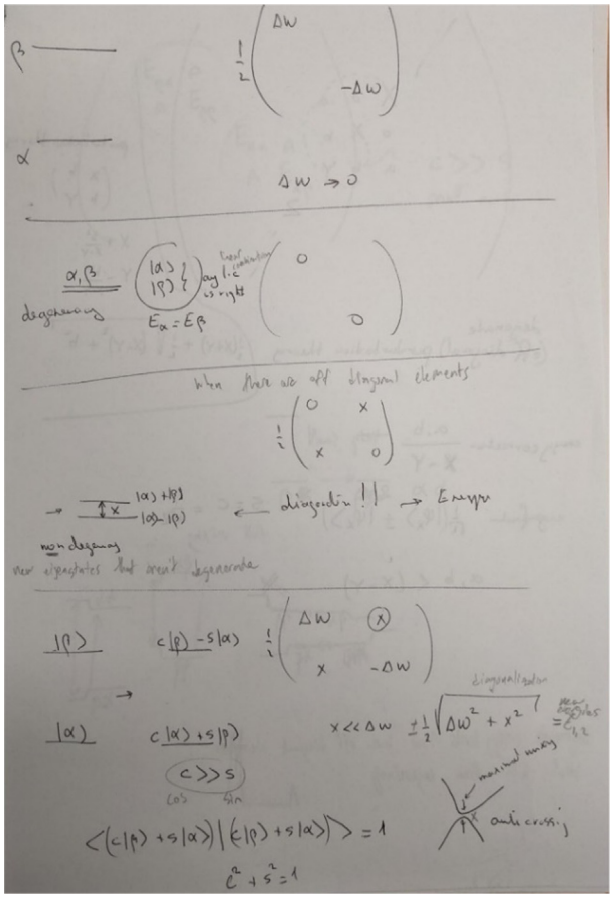
10. Ingolf Sack

Shimon was an extraordinary person and outstanding teacher. Perhaps he was the most important teacher for me, with whom I was fortunate to spend a certain period of my life in Israel, at the Weizmann Institute. Shimon had the ability to explain things that loomed only hazily on the horizon of my experimental work in solid-state NMR. This allowed him to predict early on how we would need to design the experiments to accurately determine ^{2}H–^{13}C distances with maximum signal yield. Whether it was the analytic derivation of the Hamiltonian in this specific spin-1 spin-1/2 quantum system, or tensor diagonalization in general, Shimon did this with an ease as if it were small talk. Indeed, working with Shimon had the joy, inspiration and ease of a long conversation among friends in which one learns much about the essentials of science and the meaning of life. I am forever grateful to Shimon for the time I was privileged to spend with him, which had a lasting impact on me beyond the realm of science.

11. Daphna Shimon

I'm honored to be Prof. Vega's last PhD student. When I joined his group in 2008, the interest in DNP was seeing a resurgence, and I had the great privilege of learning NMR and DNP from Shimon, while also learning DNP together. We spent many hours sitting together trying to understand the experimental data I had accumulated and to figure out how to model the spin physics of DNP when we could only simulate at most 5–6 spins. There were many days when he would come in the morning and tell me that overnight, he had thought of another way we can try and simulate the thing we were looking for. This persistence is something that I always associate with Shimon. He would never give up on trying to understand even the smallest experimental feature. The things I will most remember about Shimon are probably the things many others will remember too: how kind he was, how humble, how good a teacher, and how he always knew how to adapt his explanation of a topic to the person he was talking to. At the very beginning of my masters, I was starting to write simulations of DNP, but I did not fully understand what I was doing. One day, I was simulating a small spin system, and he had me look at the energy levels as a function of the off-resonance. He had me zoom all the way in and then asked me what I saw. He used this exercise to explain anti-crossings and state mixing. That was the day I finally under-

stood the simulations. I kept the paper, which he wrote upside down so I could read it while he was writing, and I still have it to this day. It's a joy to look back and realize how clearly he could explain complicated topics. Part of this paper is shown here.



12. Sundaresan Jayanthi

I was fortunate to be associated with Shimon during my graduate studies at the Indian Institute of Science (IISc) in Bangalore. Thanks are due to Madhu for introducing me to Shimon in 2004. While at the IISc, I had frequent email conversations about NMR with Shimon, and most of the time he responded within 24 h. He had invested time and patience in answering my NMR-related queries, and those discussions were very helpful for me in my early research and also throughout my career.

Subsequently, I joined Shimon at the Weizmann Institute as a postdoctoral student in 2010–2013. I was his last postdoctoral student who worked in a solid state NMR project. During that time, we worked closely with Asher Schmidt and Shifi Kababya, which led us to multiple train journeys to Haifa, starting early morning, utilizing the time during our journey to discuss Floquet theory and deuterium dynamics. The eight-hour computational time for a Floquet Matlab® simulation was addressed in one of those train journeys with a lot of equations, and in the following week, we could reduce the computational time to a few minutes. Whenever I was stuck with the underlying theory of deuterium dynamics and adsorption–desorption kinetics of small molecules in mesopores, he reassured me that "we are together in this project, we will understand it soon". That was more than an assurance and I realized only later, when I started my career, that the knowledge I acquired when I was with him was abundant and priceless. Whenever I reached out, he continued his support by all possible means, with no hesitation and no delay, but each time with more energy, enthusiasm and joy. He helped me tremendously in every aspect of my life, be it NMR, career, or personal life.

Shimon was such a wonderful person, a "spring of wisdom" as Asher says, a humble human being and a great scientist. His passing away has left a void impossible to fill. Yet I consider myself privileged and fortunate to have known him. The amount of cheerfulness, knowledge, care, concern, friendliness, and comfort that he has given each one around him, I hope will lead me ahead in my journey. The contagious energy and enthusiasm, when he was around, is what I would like to carry in his absence. By behaving the 'Shimon way', he taught me how to treat others, how to be humble yet competitive, ambitious but aware of our own limitations, and finally to respect everyone for what they are. I will be missing Shimon, yet Shimon will always be around.

13. Elena Vinogradov

When I was accepted to the PhD program at the Weizmann Institute I was elated and somewhat surprised. I was not sure what I would study, but I was quite sure it would not be NMR. In fact, during the admission interview I was asked about NMR and I told them, honestly: "I don't know much about it, I am not interested in it and I prefer not to answer any questions about it". Despite my *hutzpah*, I was accepted. And then, I had to take a quantum mechanics course. And I was privileged to meet the best Teacher I had ever met and one of the best people I was fortunate to encounter. Shimon's approach to teaching stunned me. He rarely gave a straight answer. He was always asking what we thought. He was actually making sure that we understood. He was always saying that he does not know/remember or only recently understood the answer. It was always "answering a question with a question", but taken to unbelievable levels of scientific curiosity. I was hooked on the discussion. On the opportunity to think. I thought to myself that it would be interesting to do a rotation in his lab. The rest "is history".

My first project was under the supervision of him and Professor Zeev Luz (another giant of NMR). The project failed, but the remnants of the simulation code came useful in the next steps. I was lucky to join Madhu and work on the PMLG experiment. The most challenging and rewarding part was the derivation of the bimodal Floquet theory and its application to describe the combined effects of MAS and periodic RF. We spent countless hours going over the equations, of course with me trying mostly to catch up with what Shimon had already understood. Many times, Shimon would come in the morning and say something like "I was thinking about it…" which would start derivations and discussions that ensued for several days. The whiteboard would be covered with formulas, and signs of "do not erase" would be written. Floquet theory described all the experiments beautifully. Not only were we able to explain experimental observations (broadenings at specific spinning frequencies) but also to predict experimental features, such as the position of the rotary lines. Moving on to less steps and expanding to a windowed version, the scaling factors, the deterioration of efficiency, everything was explained there, by the Floquet theory. To have a theory that correctly predicts experimental outcomes and to be able to confirm it by doing the actual experiment is exactly what science is about.

Shimon was always respectful of others. He was humble and always knew something wise to say (or not to say) in challenging situations. I left solid state NMR and moved to imaging. During all the years after my PhD I would call Shimon often to talk about science and life. He was always interested, even in the projects that had little to do with his own research. When DNP reached *in vivo*

imaging, we had several interesting discussions about its applications and the future of the technology. After these conversations I always felt enlightened and optimistic about science and life in general.

Without Shimon, the world is darker. Shimon, you are greatly missed.

On January 18th, 2022, Massachusetts Institute of Technology held an online tribute symposium "Remembering Shimon Vega" organized by his long-time friends and colleagues Robert Griffin, Kong Ooi Tan, Daniella Goldfarb and Lucio Frydman. This seminar is available online [3].

Shimon Vega, early days at the Weizmann Institute.

Acknowledgements

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[3] https://youtu.be/gcxP4GgotW8.