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Autobiography of Robert Benny Gerber

I was born in Ashabad, Turkemanistan, then part of the USSR, in July 1944, when the Second World War was in its final phase. My parents, who originated from a small town in Poland, narrowly escaped the holocaust by escaping into the Soviet Union at the beginning of the Nazi onslaught in 1941. My father was assigned to a construction task in Turkemanistan. Escaping from Poland saved my parents' lives, but the USSR under Stalin was a repressive state, ruled by fear. Fortunately, after the war, we were able to escape to Western Europe. Soon after the proclamation of the State of Israel my family emigrated there and it has been my home ever since. I have fond memories of growing up in Tel Aviv and of my school years there. Israel was a relatively poor country at the time, certainly by Western standards. However, education was held in high social regard and was given high priority. My impression is that now, although the country has become much more affluent, the quality of education is actually becoming more limited. I hope that things will improve soon again. My chemistry and physics teachers in high school were inspiring and charismatic personalities. They strongly influenced my choice of career. For my parents, academic education was a dream, quite unattainable for themselves when young. They encouraged me to study and gave me all possible support.

University Studies. In the Fall of 1962, I enrolled as a student of Chemistry at The Hebrew University of Jerusalem. There were 6 candidates for each slot, with a total of 60 first-year students. This shows the great interest in the physical sciences at the time. The level of students in the class was outstanding. A very high number of my class continued on to academic or other research careers. One of my classmates was Moshe Shapiro, now at the Weizmann Institute at Rehovot, and at UBC in Canada. Moshe, an outstanding theorist and a close friend, also later became one of my first collaborators. Another former classmate, Uzi Landman, is now a leading condensed-matter theorist at Georgia Tech. My friend Yehuda Haas is my colleague at The Hebrew University, and Salman Rosenwaks is on the Physics Faculty at Ben-Gurion University. Also, the records of other classes around those years are strong. The Hebrew University of Jerusalem has certainly educated a substantial number of researchers in chemistry and physics, and the impact has been international. During those years, quantum chemistry was not yet part of the undergraduate curriculum at The Hebrew University. However, several books drew my attention, in particular C.A. Coulson's inspiring "Valence", and I became interested in the subject. The late Professor Saul Patai, a distinguished physical organic chemist, thought well of my record of studies and showed interest in my future plans. He encouraged me to pursue doctoral studies with Professor C.A. Coulson at Oxford, with whom he was acquainted. At his initiative I obtained a Research Fellowship at Oxford to work with Coulson. This was extremely generous and supportive on Professor Patai's part. In the summer of 1965 I graduated from The Hebrew University, with a B.S. in Chemistry (with Excellence) and went to England for graduate studies at Oxford.

Doctoral Research at Oxford. The opportunity to work with Coulson was an elating experience for me, as well as a great challenge. Oxford was a new and completely unfamiliar world for me. Even my command of English left a great deal to be desired. Nevertheless, I enjoyed the experience greatly from the very beginning. One reason was that the University of Oxford is a very welcoming environment, positive and tolerant toward outsiders. The main factor was, however, my research advisor, Professor C.A. Coulson, FRS: a great scientist, a highly influential and leading figure in theoretical chemistry, and also a wonderful human being and perfect mentor. Coulson was extremely encouraging and supportive as well as tolerant toward my limitations as a beginner. He had the gifts of communication and of presenting subtle points simply. I loved the way he taught and explained ideas. His scope of knowledge was immense, covering fields of molecular science, physics, mathematics, and more. Actually, he was Professor of Mathematics, and his very large group reflected the diversity of his research interests. The group's location was at the Mathematical Institute at Oxford. He was immensely busy, yet always found time to help. Coulson always tried to suggest but never to impose his views. Under these circumstances I had a lot of independence from the outset, but with the benefit of advice when needed. I was fascinated by mathematical topics to which I was exposed at the Mathematical Institute. This motivated me to pursue formal theoretical rather than computational work. Coulson's approach was that both theoretical directions such as mathematical models and computational techniques are essential for progress in the field. Most people in his very diverse group actually pursued chemical topics through computational tools. Tony Joseph, my best friend at Oxford, is an example of somebody who started as a chemist and became extremely fascinated by the mathematical subjects to which we were exposed. Today, he is a highly respected mathematician at the Weizmann Institute. Before coming to Oxford, I considered working on molecular orbital theory. Soon after my arrival at the Mathematical Institute, I attended several seminars on molecular scattering theory, which was a hot topic at the time. Scattering theory has an elegant formal structure, and I decided to choose it as the subject of my thesis. I focused on properties of the adiabatic approximation for molecular collisions and pursued research that was almost entirely noncomputational. Coulson was very open minded and left the decision to me. Many members of Coulson's group chose much more computational topics and he also welcomed this. I enjoyed formal theory, and results came quite quickly. I wrote four papers on my thesis work. Coulson was very positive on my work and there were other encouraging indications. After about a year at Oxford, I was elected for a Senior Scholarship at Pembroke College. Later, I got the (second) Senior Mathematical Prize, awarded for the most outstanding thesis of the year. I was happy with these achievements, and thought to continue in the same direction. Only much later did I understand the downside of this type of research: The results were not of substantial significance for the chemical community, where I wanted to perform my future research. I obtained the Ph.D. after 3 years at Oxford. With Coulson's generous support I got several very attractive offers for postdoctoral positions. I accepted the offer of Professor Karplus at Harvard. Of special interest to me was his work on reactive molecular collisions.

Postdoctoral Research at Harvard. I arrived at Harvard in August 1968, where I found a wonderful, intellectually stimulating research environment, yet completely different in ambience and points of strength from the Mathematical Institute at Oxford.

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This was an exciting and very intense time in Chemical Physics in general, and in molecular reaction dynamics in particular; Harvard was at the very epicenter of it all. Harvard had it all: Great leaders in the field, both in theory and experiment, a community of exceptionally bright students and postdocs; and an intense atmosphere, conducive to discussions. It was incredibly stimulating to be there at the time and to pursue research in the field. I felt that I was learning daily from discussions. The theory students and postdocs had their offices at Prince House, a former old private residence converted for the purpose. Students there were doing their research at all times, day or night. My office mates were Millard Alexander (now at Maryland) and Jimmie Doll (at Brown). I had many discussions with them and also with other Prince House dwellers, including Barry Honig, Paul Brumer, Hersh Rabitz, and—at a later time—Klaus Schulten. I learned a lot from Bill Miller, then a Junior Fellow, and Bill Reinhardt, then Assistant Professor. Both were very approachable, extremely knowledgeable, and willing to share their insights.

In leading his research group, Martin Karplus put the emphasis on a selected range of topics of major chemical importance. He already began his move toward computational studies of biological molecules. Many people in the group at that time worked on chemical reaction dynamics, either on calculations of potential energy surfaces or on classical trajectory simulations of molecular collisions. They were, by the standards at the time, computationally intensive projects. In this respect, there was a very big difference between the Coulson and the Karplus groups. I found myself at a major disadvantage, lacking experience in calculations and still very fond of analytical methods. I decided, perhaps wrongly, to carry on with analytical theory. Martin Karplus understood and agreed, though clearly this was not the focus of the group. During my year at Harvard, I published 3 papers with my mentor, all noncomputational in content. One of these papers I consider a very good one. It deals with the question of whether one can obtain also the phase of the scattering amplitude from the measured differential cross section. This topic is of fundamental interest in the context of the inversion problem, in which the aim is to determine the interaction potential from scattering data. My approach was to use the property of unitarity, satisfied universally by scattering amplitudes, which leads to an equation linking the phase to the measurable cross section. The paper obtained conditions for uniqueness of the solution for the phase and introduced convergent algorithms for determining the solution. From an analytic-mathematical point of view, the results are as elegant as any I was able to obtain in my career. I even received nice comments on the paper from the great R.G. Newton, a maestro of scattering theory. However, the paper was not of much chemical interest. I was determined to go back home after one year as postdoc. I wanted to see my aging parents. I published three papers from that period but my most important gain from Harvard was the "live wire" research atmosphere in the group and the department, and above all the interactions, discussions, and contacts with a host of brilliant people. Several of them have remained my good friends, and quite a few have made a major impact in chemistry.

Weizmann Institute of Science, 1969−75. I arrived at the Weizmann Institute in September 1969. It has a pleasant campus, located at the small town of Rehovot. The Weizmann has a graduate school but does not admit undergraduates. The faculty have only research as their obligation, with teaching in the graduate school being optional. The Chemical Physics Department, headed by Shneior Lifson, had capable scientists but was rather small and, at least in the beginning, had no people with whom my research interests overlapped. There were almost no seminars in my research direction. A great asset was Professor Shneior Lifson, a very wise scientist and deep thinker, with whom I loved to discuss. Lifson, together with his outstanding student, Arieh Warshel, were working on the development of a code for determining reliable empirical force fields for organic and biological molecules. However, I failed to take full advantage of my stay at the Weizmann, since I worked in isolation, on analytical-mathematical problems.

On the other hand, this was a wonderful period in my personal life. At the Weizmann I met Helene Grigoriu. She was born in Romania but raised in France. She did research in organic chemistry of natural products in the laboratory of M. Fetizon in Orsay, and there obtained a graduate degree, then came to Israel. We fell in love and after a courtship of over a year were married in 1972. Since then, Helene has provided immense support of my career. She decided to give up efforts for a career of her own in Science, and converted to Pharmacy.

Fulfillment in personal life could not, however, provide a relief from my growing concern about tenure. Only during the second half of my six-year appointment did I begin to emerge from stagnation in my research program. One very positive development was Lifson's initiative to expand the Department. I benefited in particular from the arrival of Moshe Shapiro, who joined the faculty. I knew Moshe from our undergraduate days, we shared research interests and we interacted very well. We began to work jointly on an inversion method for the direct determination of interatomic potentials from scattering data. Another move out of stagnation came when I became interested in recruiting graduate students at about the same time. My first three research students were enrolled at the Weizmann, although they completed their doctorates after I moved to Jerusalem. The third among these, Max Berkowitz, was a deep thinker, with sharp physical intuition. I enjoyed working with him and I was now convinced that, at least for me, interaction with students can be immensely rewarding and stimulating. Research became much more lively and dynamical in this interactive manner. All this happened too late for rescuing my career at the Weizmann. I was, however, rescued by an unexpected offer: The Hebrew University of Jerusalem decided to recruit two young theorists and made me an offer as an (untenured) Associate Professor. I accepted without hesitation.

Hebrew University of Jerusalem. When I arrived in Jerusalem in 1976, the nature of my research and the approach I took were strongly different from previous periods. Above all, The Hebrew University was a great environment for recruiting outstanding research students, which by then I was eager to have. I still had Max Berkowitz coming to work with me from the Weizmann Institute for part of his doctorate. In my two years at Jerusalem, I was fortunate to recruit three students: Tamar Yinnon, Victoria Buch, and Ron Elber. These four students "walked on water" when it came to research. Work with each of them was rewarding and inspiring. Far from just doing calculations assigned to them, they contributed ideas and worked as creative young researchers. A few years after her doctorate, Tamar Yinnon chose not to continue in science, due to personal reasons. Her work on molecular scattering from surfaces had a substantial impact. Max Berkowitz (whose doctorate was on vibrational relaxation of molecules in matrices); Victoria Buch (who worked on scattering theory, on time-dependent mean field methods for molecular dynamics, and on dynamical processes in clusters); and Ron Elber (whose doctorate was on energy transfer and dissociation in molecule−

surface collisions) all went on to become very successful scientists of international renown in their respective fields. To my good fortune, very motivated and creative research students joined my group in subsequent years, and the group is now larger in number than ever before. At that stage, I recognized at last that my research could benefit greatly by recruiting talented postdoctoral research fellows. I find the influence and ideas from other groups that postdocs bring to our research group extremely valuable. Many of the postdocs who joined my group did terrific research during their stay and went on to highly successful careers in academia and elsewhere. I believe that the research environment at The Hebrew University contributed in attracting postdoctoral fellows from overseas. In 1982, the Fritz Haber Research Center was established at The Hebrew University, with R.D. Levine as founding director. The first emphasis was molecular reaction dynamics. Later, the center expanded to cover all areas of theoretical chemistry. The Fritz Haber Center was conducive in creating a critical mass of researchers in theoretical and computational chemistry.

Another major change in my research direction after I came to The Hebrew University was that I became very motivated to pursue theoretical research strongly connected to experiment. This began during a visit in 1975 to the Max Planck Institute in Göttingen, Germany, at the invitation of Professor Udo Buck, a world-class leader in molecular beam scattering. Udo has become a close friend and collaborator of many years standing. Work with him was always intellectually stimulating due to his insights and command of the field, and also personally very gratifying. The first visit to Göttingen was a revelation to me: I visited state-of-the-art laboratories in molecular beam scattering, and realized that modern experiments in chemical physics can be highly sophisticated, elegant, and challenging, and that contact with such experiments can provide special motivation and a sense of purpose for theory. The work with Udo Buck that developed after this visit is a type of research that I greatly cherish: Theoretical−experimental projects, in which a problem of interest is tackled jointly by a theoretical and an experimental group. Later on, I had the great benefit of such collaboration with several other distinguished experimentalists. In any case, work strongly related to experiment has become one of the main themes of my research.

Cooperation with other theoretical groups has also become a very important aspect of my research. At the Weizmann I cooperated with my colleagues Moshe Shapiro and Viktor Yakhot. In Jerusalem, I interacted in particular with Ronnie Kosloff and Avinoam Ben-Shaul, as well as with others. Long-standing collaborations that have lasted for many years with Mark Ratner and with Don Kouri, having begun during visits they made to The Hebrew University. Such cooperations with other groups have been, and still are, a cornerstone of my research.

Finally, I found it very important that The Hebrew University also has undergraduates, with many chemistry majors. I found that I appreciate teaching and love it. Twice, I won awards for long-standing excellence in teaching, which is very close to my heart. On the whole, I prefer a university to a research institute as a professional home.

I had an increasingly positive feeling about my progress since I came to Jerusalem. I have expanded my research interests and directions. I have had almost continuously a wonderful group. Some of our work has had impact on several subjects, and as of 1977 or so, I was increasingly asked to speak at a good number of international meetings. This was recognized by the university. Two years after my arrival, I was granted tenure, and after two more years I was promoted to Full Professor. The Hebrew University has been to me since then a professional home that I like and appreciate. An important additional reason is that all our family, including my wife Helene, and our son David, like Jerusalem. It is a very special, fascinating, interesting, and complicated city.

Dual Position: Hebrew University of Jerusalem and University of California at Irvine. In 1990, I got a second professional home, in addition to The Hebrew University. I was offered a permanent, part-time position at the University of California at Irvine, and gladly accepted it. In this position, I spend a period of 3 months each year at UCI, doing research there, and teaching for the quarter. This arrangement offered me an opportunity to expand my activities, interact with more research groups, find new collaborators and refresh my research directions. This proved to work out very well for me. There is, admittedly, a major effort in making the very long trip, but it is rewarding. Upon joining UCI, I found a very young and fast-growing department, very different from The Hebrew University. One remarkable characteristic of UCI, at least until now, is the ongoing recruitment of new faculty. I had a very fruitful cooperation with Ara Apkarian on photochemistry of small molecules in rare-gas solids even before I joined UCI. His has been a leading laboratory on a topic that has relatively few champions, and that I find very interesting. Another very early and successful cooperation was with Doug Mills, a distinguished condensed matter theorist at the physics department. Our cooperation was on hydrogen at metallic surfaces. A new research direction to me that I owe completely to UCI is atmospheric chemistry. I became interested in the field thanks to stimulating discussions with Barbara Finlayson-Pitts. I have become a member of an NSF-sponsored institute in atmospheric chemistry, and have cooperated with several of my colleagues in this framework, to my great benefit.

In the beginning of my affiliation with UCI several members of my group at The Hebrew University would travel back and forth with me. This is justifiable for outstanding postdocs and students who can respond to the challenge and take advantage of the experience. The outstanding members of this “travelling group” benefited from the experience and it contributed to their scientific growth. Present Visa issues make this, however, difficult for those who are not US citizens.

In time, I was able to get also a small number of “Irvine-based” postdocs and students. Some of them were shared or joint with other UCI faculty. Several students chose to work independently during my long absences from UCI and were very successful in their research.

My work on most of my research topics spanned quite a few years. The following is an account of evolution of my main research projects and the collaborations that shaped several of them.

Inversion of Scattering Data. The aim of this research direction is to determine intermolecular potentials by direct inversion of measured differential cross sections, free of assumptions of parametrized forms. I made a first contribution to this problem as a postdoc with M. Karplus (in 1968) by showing that the phase of the scattering amplitude can be obtained from the differential cross-section, by very effective algorithms applied to the unitarity equation. Several years later, working in cooperation with Moshe Shapiro, we expanded this into a full inversion method to determine the potential function from the differential cross section for atom−atom scattering. The method first constructs the scattering amplitude, including the phase, from the cross section. Then, the phase-shifts are readily computed from the scattering amplitude and used to construct the potential. I found it very exciting nearly two years later when the inversion method due to Moshe Shapiro and myself was applied to differential cross sections for He−Ne scattering, measured at high resolution by Udo Buck and his student. Many tests other than scattering show that indeed the inverted potential is of high accuracy. When Victoria Buch, now Professor at The Hebrew University, joined my group as a highly gifted research student, she proceeded to develop an inversion method for rotationally inelastic scattering, in which case the objective is to determine the anisotropic interaction potential between an atom and a molecule. We cooperated on this with Udo Buck and his group, who carried out the pioneering experiments. Again, the inversion method proved very successful. The application to Udo Buck's elastic and inelastic cross sections for Ne + D_2 led to the determination of a very accurate anisotropic potential. Work on inversion involved very stimulating interactions with experiment and the development of interesting algorithms. There was interest in the community, reflected by the publication of results in *Phys. Rev. Lett.*, etc. However, the inversion method has not proved an important tool. The emergence of improved fitting methods, despite their disadvantages, and above all the advent of reliable ab initio methods for computing interaction potentials carried the day, and these became the most important tools for obtaining intermolecular potentials. The inversion methods have, however, resulted in important insights by throwing light on the relation between scattering data and the underlying interaction potentials.

Low-temperature Chemistry. ***Photochemical Reactions in Matrices and Clusters.*** This has been a field that stimulated my research projects for many years, giving rise to a succession of challenging problems in very low temperature systems where frequently surprising effects are found.

A first problem in this field in which I became involved was that of vibrational relaxation of diatomic molecules in noble gas matrices. Experiments by Legay and his group in Orsay, France, and by Brus and Bondybey—then at Bell Laboratories—showed very surprising effects in the case of hydrides. The widely accepted multiphonon model for vibrational relaxation in solids could not explain the experimental isotope effect (HX(v = 1) was found to relax much faster than DX(v = 1)), the temperature dependence (much weaker than expected from multiphonon models), and the relaxation time scales (much faster than previously estimated). Together with my then student Max Berkowitz, we developed a quantitative model for the relaxation process in which the dominant receiving modes were assumed to be localized modes in the impurity cage. For hydrides, the rotational mode was predicted to be the main receiving mode. Another model in this spirit was suggested by Metiu and Freed. The "local modes" based model that we put forward (1977, 1979) was well received in the field and was used by several experimental and theoretical groups in the interpretation of their findings.

I returned to another topic of the field of matrix processes in the late 1980s. V.A. Apkarian at the University of California at Irvine had embarked on very interesting experiments of photodissociation of diatomic molecules embedded in noble-gas crystals. I felt that classical molecular dynamics simulations could provide detailed atomic-level insights into these processes, including issues such as the probabilities of cage exit by the photofragments and the mechanisms of cage exit. I began to cooperate with Apkarian on this topic, with the participation of Roger Alimi, a very capable research student in my group. Examples of systems that were explored were HI@ (solid Xe) and F_2@ (solid Ar). Soon I met another leading experimentalist working in this field, Klaus Schwentner, of the Free University, Berlin. This also led a very fruitful long-term cooperation. Among useful insights that have emerged at this stage is the distinction between "direct" and "delayed" cage exit, with criteria that govern the relative yields of these different mechanisms. The molecular dynamics simulations thus were successful in providing some understanding of the processes, and the interpretation of certain experiments. However, it was obvious that they also had limitations. Particularly severe was the limitation that classical molecular dynamics does not include nonadiabatic transitions and thus cannot describe at all recombination onto the electronic ground state, one of the most fundamental processes in these systems.

The first nonadiabatic simulations of photochemistry in matrices were carried out by the group of Professor H. Gabriel in Berlin. This was followed shortly afterward by studies from Coker and Batista at Boston University and by our group. The development of the semiclassical and nonadiabatic simulation algorithm for photochemistry in solids in our group is entirely the work of Anna Krylov, a highly talented research student at the time, and now Professor at USC. The approach she employed for the nonadiabatic transitions was Tully's celebrated "surface hopping". However, the application for these systems, in which many potential energy surfaces play a role, is highly complex and challenging. Anna Krylov was able to throw light on the mechanisms and time scales of recombination following photolysis of HCl in solid argon and on the competition between cage exit by the H atom and recombination.

A little over 10 years ago came a development that opened for my group new directions in the field of matrix photochemistry and catalyzed new rewarding cooperations. A multi-investigator project, based at the Free University of Berlin, was then awarded by the DFG, the German Research Foundation. The grant, still in effect, is for research on "Analysis and Control of Ultrafast Reactions". Such funding is relatively long-term, and there is strong emphasis on cooperation. Thanks to my friends and colleagues in Berlin, I am included as a participant. My part of the project deals with ultrafast photochemical processes in matrices. From the outset I have had a very enjoyable cooperation with Joern Manz, who pursues quantum dynamics models, as well as with Klaus Schwentner, who carries out pump−probe femtosecond pulsed laser experiments. Oliver Kühn of Manz's group, Dr. M. Korolkov of Belarus, and Masha Niv and Arik Cohen of my group played pivotal roles in the project and cooperation. An interesting set of results describe the effect of different quantum numbers of the diatomic molecule (spin, orbital angular momentum) upon the process. Possibly the most interesting result is the "ultrafast spin flip," a conversion from singlet to triplet taking place on a subpicosecond time scale in the photolysis of F_2@Ar and of FCl@Ar. This, of course, is surprising for a light atom such as fluorine, which has a small spin−orbit coupling interaction. The effect was confirmed experimentally by Schwentner and his group and is among the surprises that emerge from photochemistry at low temperatures. I am quite convinced that cryogenic chemistry has many additional surprises in store.

Remarkable progress in experimental techniques allowed exploration of photochemical reactions of the above type in finite clusters, in molecular beam conditions. We were very stimulated by the findings of Curt Wittig, Udo Buck, Benoit Soep, and several other groups, who built this research topic during the past two decades. One question of interest is: how do processes in clusters depend on the size of the system, and when does the effect approach the behavior for an extended solid? Alberto Garcia-Vela, a postdoc from Spain, predicted several interesting manifestations of a "cage effect" for clusters that have but a single "solvent" atom influencing the reaction. In cooperation with Curt Wittig and his group at USC, we found that theory and experiment point to a "single-atom cage effect" in the photolysis of HBr in Ar•••HBr. Cage effects in clusters having one or two solvation layers can be very strong, approaching the behavior for the solid. This has emerged from work by Roger Alimi, Masha Niv, Burkhard Schmidt, and others of our group, in studies that included cooperation with experiments by Udo Buck and co-workers. One interesting result from such a joint theoretical−experimental study is that photolysis of HCl absorbed at the surface of an Ar_n cluster involves a pronounced cage effect. When Anne McCoy joined our group as postdoc, she did important work on photochemistry in hydrogen-bonded clusters (HCl dimer) in which internal reactions occur. Jeremy Harvey made another valuable contribution to the field in his work on photoexcitation of water clusters. This field is at an early stage of development but is very exciting.

Molecular Collisions with Surfaces. In the late 1970s, interest in molecular beam scattering from surfaces as a tool for exploring molecule−surface interactions, had begun to grow rapidly. I was attracted to the field because of its potential importance and richness, but also because I felt that my experience with gas-phase scattering could serve as a useful background for the relatively new research area. Our first contributions were to the development of approximate methods for computing scattering distributions for molecular collisions with crystalline surfaces. We dealt with diffraction scattering (by a Sudden approximation), with rotationally inelastic scattering (again, a Sudden type approximation was developed), and with vibrationally inelastic scattering (a Sudden approximation for rotation, combined with a perturbation method for the vibrational transitions). In all three cases, the approximations we developed were well received in the field and proved useful in a range of applications by other groups. The key player in most of this work was Tamar Yinnon, a very motivated and enthusiastic research student. We cooperated with Professor John Murrell, who visited from Sussex in England, on the diffractive scattering work. A visit of D.J. Kouri, of the University of Houston, was the start of a long-term and very fruitful cooperation. We benefited greatly from Don Kouri's mastery of scattering theory.

A few years afterward, in the mid-1980s, our interest in this field shifted to the use of atom scattering to study defects on crystalline surfaces, and disordered surfaces in general. We developed approximations for the scattering distributions. However, this research gained great impetus when I began to interact with my Hebrew University colleague Ronnie Kosloff and used his very powerful quantum wavepacket propagation method. Very exciting also was the cooperation that we had established with the leading experimental group of Professor G. Comsa of KFA, Jülich, Germany. Joint theoretical−experimental studies shed light on structural properties of defects on surfaces (adsorbates, vacancies) and also of structurally disordered surfaces. Much of the work on this by our group was done by Tamar Yinnon, and later also by Daniel Lidar, then a graduate student (now Professor at USC). I recall with great fondness our joint work on this with Professor Guiseppe ("Peppino") Petrella of Bari, Italy, who visited The Hebrew University several times. He was very enthusiastic, dedicated, and extremely kind and helpful. His untimely death was a great shock to members of my group who liked him a lot. Another fruitful cooperation in this field, specifically on scattering from models of disordered surfaces, was with Herschel Rabitz, Joel Gersten, and D.K. Dacol, during a two-months sabbatical I spent in Princeton in 1982.

The work on atom scattering from disordered surfaces was met with some interest at the time. However, it became clear to us in several years' time that interest in the field had waned to a large extent. Probably, this was due to the development of STM experiments, which had some advantages over atom scattering. This is certainly part of progress in science, particularly in chemical physics. Technology creates research areas and can also bring about their decline.

Our interest in vibrationally and rotationally inelastic scattering led to an effort of modeling a more challenging process in molecule−surface scattering; excitation of electron−hole pairs, in the case of a metallic surface. It was stimulating to try and provide a quantitative model for this process with two of the most fruitful collaborators that I worked with over the years: Abe Nitzan (Tel Aviv) and Mark Ratner (Northwestern). We obtained some useful insights, but even today relatively little is known about such processes.

In the 1980s we became very fascinated by pioneering experiments by Aviv Amirav of Tel Aviv University and his then student Eli Kolodney (now Professot at the Technion, Israel Institute of Technology). Amirav's group carried out pioneering experiments, in which they bombarded single-crystal surfaces (MgO, diamond, etc.) with very energetic beams of molecules such as I_2. They were able to measure in these experiments dissociation probabilities in single molecule−surface collisions, a challenge for rigorous microscopic modeling of a reaction at the vacuum−solid interface. Ron Elber, then my student, and I joined Amirav and Kolodney in this project to model the process and provide insights. This was a truly wonderful experimental−theoretical cooperation. We found that theory can account for the experimental dissociation probabilities as a function of energy; that excitation of the I_2 rotation upon impact is a key factor in the dissociation; and that impact of I_2 upon the surfaces creates a shock wave, traveling from the surface into the bulk. Rob Elber has emerged from the very outset as an outstanding young theorist, equally at home with developing models, writing a simulation code, or interacting with the experimentalists. Today he is Professor at the University of Texas at Austin.

Around 1990, I heard of a very ambitious and very elegant research program by Professor Gil Nathanson at the University of Wisconsin to explore scattering of molecules from liquid surfaces. Impressed by the progress he has made, we embarked on research efforts to study the scattering processes by classical molecular dynamics simulations. We formed a cooperation with Nathanson's group, which was very rewarding. We first pursued Xe scattering from liquid squalane, a hydrocarbon. This was explored by Nuphar Lipkin, a postdoc in our group, in cooperation with Nimrod Moiseyev, a close friend and colleague from the Technion. Then, David Chase, a graduate student of my group, undertook the challenge of scattering of atoms from liquid indium. The primary goal of scattering of atoms from liquid metals, in my view, is the unraveling of structural and dynamical properties of liquid metal surfaces, of which relatively little is known. The joint study on this with the Nathanson group provided some very useful information. For example, embedded atom potentials proved successful in modeling the liquid indium surface. However, this is only a modest step forward in a difficult field. My feeling is that atom scattering from liquid surfaces deserves many more extensive studies in future. Part of my current research in atmospheric chemistry is on processes at the gas−water interface. This will be discussed later.

The VSCF Method and the Vibrational Spectroscopy of Biological Molecules and Other Large Clusters. I became interested in the problem of coupled anharmonic vibrations of polyatomic molecules in the midseventies, having been exposed to the growing interest in vibrational excitations of polyatomic molecules, and their relation to intramolecular vibrational energy redistribution. Mark Ratner visited The Hebrew University in 1977, and we readily embarked on a cooperation that turned out to be a long-term one, very enjoyable and productive. We formulated an approximation for coupled-mode anharmonic systems, in which the total wavefunciton was assumed to be a product of wave functions associated with each mode. A variational approach leads to equations for the wave functions and energy levels. This separable (Hartree) approximation is the simplest level of what came to known as the vibrational self-consistent field (VSCF) method. Ratner and I published our results, including simple test applications for models, in 1979. We were not, however, the first. This credit goes to Joel Bowman, who published in 1978. Several other groups around that time also independently pursued this subject, or related approximations. For several years, the progress we made was rather slow. We did not have at hand a practical method for any but the smallest polyatomics, and applications depended on having potentials in analytic form. An important insight that emerged was that the choice of the vibrational modes (coordinates) can substantially affect the results. Work in 1986 by Zlatko Bacic, then a postdoc at The Hebrew University, and in cooperation with Mark Ratner showed that description of the large amplitude vibrations in the HCN ↔ HNC system can be accomplished by VSCF in spheroidal coordinates. In a study with Rick Roth, then a graduate student of Mark Ratner, light was thrown on the relative merits of local modes, normal modes, and hyperspherical coordinates. Tom Horn, who joined us as a postdoc in Jerusalem, explored VSCF for a range of very floppy systems, such as the van der Waals clusters I_2He, $XeHe_2$, and $(CO_2)Ar$. Choice of geometrically motivated coordinates in each case yielded excellent results in VSCF calculations, and these were greatly superior to VSCF using the standard normal coordinates, for these highly floppy, unusual systems.

However, the whole direction of our VSCF studies, their usefulness to the field, and the algorithms for implementing them changed drastically from the late 1990s. Joon Jung joined my group as a graduate student at UCI. We decided then to develop extensions of VSCF, which can be useful for much larger polyatomics and can be conveniently applicable for realistic systems. Compromises had to be made for tailoring a method that is effective and practical for the large realistic systems. An obvious first choice was to build the algorithms for normal modes, which are computationally convenient and for which VSCF separately works well for the great majority of systems, accepting that these coordinates fail for extremely floppy systems.

The computational power of VSCF in normal coordinates was demonstrated in calculations of the fundamental excitation energies and vibrational wave functions of a small protein. The calculations were done by Adrian Roitberg, who spent postdoctoral time with me and with Mark Ratner, and were done in cooperation with Ron Elber, whose biomolecular code package MOIL was highly useful in the project. As a first approximate calculation of anharmonic vibrational wave functions of a protein (BPTI in this case), it proved stimulating to the community and our paper was accepted in *Science*. However, the limitations of such VSCF calculations also became evident from this effort. The code required a simple and unrealistic potential surface. Also, it became evident that the VSCF approximation based on separability could not provide sufficient accuracy, for the experimental state of the art. Joon Jung and I introduced two major improvements: In our work, we used second-order perturbation theory to include the effect of nonseparability of the vibrational wave functions (we called the method CC-VSCF—a somewhat confusing name. A better name would have been VSCF-PT2, with PT2 standing for second-order perturbation theory). Experience in applications since then has confirmed that in the great majority of cases, VSCF-PT2 does have the necessary level of accuracy for useful comparisons with experiments. Equally important, it is sufficiently convenient computationally to allow for calculations for systems with a substantial number of degrees of freedom. Thus, VSCF-PT2 promised a reasonable range of applications. For example, our first paper on VSCF-PT2 presented spectroscopic calculations for $(H_2O)_n$, up to $n = 8$. In the work with Jung, we also introduced an effective new method for representing (approximate) the potential surface. The method represents the potential by a sum of single-mode terms and of interactions between pairs of normal modes, neglecting interactions between triplets or more normal modes. This allows for efficient grid-representation of potentials of high dimensionality and again was found to work well for the great majority of application systems. With all these ingredients, and with the code that Joon Jung developed, we felt that a method of wide applicability and computational power was at hand.

At that stage, Dr. Galina Chaban, who got her doctorate with Mark Gordon at Iowa State, joined my group as a postdoc. She had great knowledge of ab initio methods and recognized the desirability of pursuing anharmonic calculations by directly employing ab initio potential surface points, avoiding fitting and analytic representations. A combined effort by Galina Chaban and Joon Jung resulted in an algorithm for anharmonic calculations of polyatomic systems that combines ab initio methods for the potential with the VSCF-PT2 algorithm for the vibrations. A range of very encouraging applications, including, for example, glycine and the glycine−H_2O complex, emerged in a relatively short time. Professor M.S. Gordon and Dr. Michael Schmidt have incorporated the VSCF algorithms into the GAMESS suite of electronic structure programs. In years to follow, the Gordon group made important extensions and improvements to the VSCF methodology. The availability of the VSCF codes in GAMESS lent major impetus to applications of the method. In subsequent years, a substantial number of VSCF applications (including the VSCF-PT2 level) were presented by several theoretical and experimental groups. VSCF codes in the variants we developed are also incorporated in the MOLPRO suite of programs (work of Dr. G. Rahut). We have continued to pursue extensions of the VSCF methods, and this remains an important subject of our work. Working with Professor Nikita Matsunaga of Long Island University, who visited our group at UCI, and in cooperation with Galina Chaban, we developed extensions for cases where vibrational degeneracies cause significant effects (our extension deals only with 1:1 resonances). In another direction, work by Liat Pele, a student currently in our group, and Dr. Brina Brauer, a postdoc, led to greatly accelerated VSCF algorithms. The scaling of the computational effort with N, the number of modes, is improved by a factor of N^3 for large N for VSCF-PT2. This opens possibilities of VSCF-PT2 calculations with reasonably reliable potentials for, for example, small peptides, which is a major advance in the field.

We find applications to spectroscopy of interesting specific systems as appealing as the methodological and algorithmic issues. Projects pursued jointly with an experimental spectroscopy group, where we use VSCF calculations to help in the interpretation, have proved particularly rewarding. One direction we have focused on is the spectroscopy of biological molecules. Important contributions were made for such systems by Sue Gregurick, Galina Chaban, Joon Jung, Brina Brauer, Adeyemi Adesokan, and Dorit Shemesh. Systems to which we made some contributions include amino acids, NMA, small peptides, glucose, complexes of nucleic acid basis, and the chromophore of the photoactive yellow protein (PYP). We had very stimulating interactions with pioneering experimental groups that include M.S. de Vries (UCSB), O. Dopfer (Technical University of Berlin), and Rich Mathies (UC Berkeley). Many of the applications have focused on the novel, high-resolution experiments on biological molecules in high vacuum. The interaction with the Mathies group on Raman spectroscopy of intermediates in the PYP photocycle raises the challenge of dealing with vibrational spectroscopy in condensed phases by VSCF calculations restricted to a chromophore and using suitable mimics of the environment. Results for PYP are very encouraging for this.

The work on anharmonic vibrational spectroscopy has received more community interest than any other subject I have pursued. I have a strong impression that with further experimental and theoretical progress, vibrational spectroscopy has the potential to become a far more important tool in studying biological molecules. Developing large-molecule spectroscopy to such a level is an exciting challenge for the future.

Mean-field Methods for Quantum Dynamics of Polyatomic Systems. In 1981/2 I spent a sabbatical at Northwestern University, which I remember as a productive and stimulating period. I embarked on a new project, jointly with Mark Ratner, to develop new quantum mechanical approximations for dynamics of systems of multiple degrees of freedom. We considered the time-dependent self-consistent field (TDSCF) approximation, proposed formally in the early years of quantum mechanics, and adopted it for the dynamics of polyatomic systems. Victoria Buch, then a graduate student, played a key role in the project and was able to implement the method quickly. The method was applied to models of predissociation dynamics of van der Waals clusters. Cooperation with George Schatz resulted in several interesting simulations of the dynamics of these processes in time. A lovely application of TDSCF was the work of Anne McCoy on resonances in the photodetachment of $ClHCl^-$. The TDSCF method met with some interest but was not practical for large systems. Also, we could not find systematic useful methods for providing corrections to improve the accuracy. This, I should say, was accomplished years later by H.D. Meyer and the Heidelberg group, in their MCTDH (multi configuration time dependent hartree) algorithm. However, the powerful MCTDH method is computationally very demanding. TDSCF served as a starting point for deriving simpler, more applicable methods, such as mixed quantum/classical algorithms for dynamics, in which only a few degrees of freedom are treated quantitatively.

Several years later, I returned to this topic, with the aim of finding a simpler quantum approximation than TDSCF, which would be practical for large systems. In 1995, I was joined by Pavel Jungwirth from Prague as a postdoc. He proved a very prolific and capable researcher, who shouldered this problem. The method we developed, the classical separable potential (CSP) approach, uses classical approximations to compute the mean field potentials that are employed in the quantum dynamics equations. The CSP method proved indeed applicable for large systems. Pavel Jungwirth, interacting also with Erick Fredj, a research student of mine, has successfully produced a range of interesting applications, especially for molecules in large cryogenic clusters. However, CSP - just like TDSCF - was limited by not having the option of useful corrections, beyond the basic level.

Quantum dynamics of multidimensional systems are a fundamental challenge, and there will be a need for new improved approximation methods. I believe that CSP may have a useful role to play, perhaps as a starting point improved by some corrections.

Mechanisms and Rates of Processes in Atmospheric Chemistry. I entered this field thanks to the vibrant activity in atmospheric chemistry at UCI. It began when my colleague Barbara Finlayson-Pitts told me of her very interesting results on the reactions of salt aerosols with O_3 and with OH. Donald Dubdab, of Engineering at UCI, pursued the kinetic modeling of Barbara's experiments, and in their analyses it seemed that the contributions of the aerosol interface were extremely important and had to be included. This motivated me and others to pursue molecular-level understanding of the special role of the surface. A very interactive and enthusiastic cooperation of several investigators came into being including Finlayson-Pitts, Donald Dubdab, myself, Pavel Jungwirth (who visited me then from Prague), and Doug Tobias, our colleague of Chemistry at UCI, a great expert on molecular dynamics simulations. The results showed that Cl^- ions (and larger halide ions) have a partial preference for the interface, compared with the bulk of the aerosol. The results suggested a mechanism for the role of the interface and led to a paper in *Science* in 2000 that became quite influential since then. Doug Tobias and Pavel Jungwirth have continued to explore in depth the issue of "surface preference" by anions, and this direction has had a major impact. Fascinated by the richness of open problems in atmospheric chemistry, I have continued since then to work extensively in this field. Much of the research I have pursued on atmospheric chemistry topics is in cooperation with the very stimulating community of my UCI colleagues in this field: Barbara Finlayson-Pitts, Doug Tobias, Donald Dubdab, and Sergey Nizkorodov. I have also cooperated with international groups affiliated with the atmospheric project at UCI: Pavel Jungwirth and Martina Roeselova of Prague, Leon Phillips of New Zealand. Yifat Miller, a graduate student in Jerusalem, chose atmospheric chemistry for the field of her doctorate. A very prolific and enthusiastic student, she cooperated very extensively with researchers at UCI, and also with Professor Veronica Vaida of the University of Colorado. Mike Kamboures joined my group at UCI as postdoc for two years and played a key role in the UCI cooperation. Dr. Bosilyka Njegic is pursuing such collaborative work now. The focus of my work in atmospheric chemistry now is the study of atmospheric reactions of NO_x molecules and related species at water interfaces. The direction is rich in promise, and we intend to pursue it actively.

Novel Molecules of the Noble Gases. ***New Chemistry at Low Temperatures.*** This is a research direction that I am very excited about. It involves the puzzle of surprising and exotic types of chemical bonding, the challenge of predicting the existence of new molecules, and working closely with experimentalists to help in their preparation and identification. For my involvement in this field I am indebted to Professor Markku Räsänen and members of his group at the University of Helsinki in Finland. Dr. Jan Lundell, also got his doctorate with Räsänen, spent postdoctoral time in my group in Jerusalem, and has kept in close contact with us ever since. He called my attention to seminal work by the Räsänen group, in which a new family of noble gas molecules was discovered. These molecules have the form HNgY, where Ng is a noble gas atom and Y is an electronegative atom or group of atoms. As it transpires, the nature of the bonding corresponds to $(\text{H}-\text{Ng})^{+\delta}\ \text{Y}^{-\delta}$, with the bonding between $(\text{H-Ng})^{t\delta}$ and $\text{Y}^{-\delta}$ being largely ionic, while the H−Ng bond is essentially covalent. The molecules are most typically formed by photolysis of H Ψ in the matrix of Ng, followed by an annealing process. Together with research student Masha Niv, Arik Cohen, and Zsolt Bihary, we explored the formation mechanisms of the new molecules, both directly in photochemistry and in a delayed, thermal process at the annealing stage after the photolysis. We have established a very stimulating cooperation with Markku Räsänen and members of his superb team, especially Jan Lundell (now Professor at the University of Jyvaskyla), Mika Pattersson (also at the same university), and Leonid Khriachtchev. In some cases our anharmonic VSCF calculations helped in the identification and characterization of the species, and sometimes our analysis threw light on the formation mechanism of the molecule, the role of the matrix, and the structure of the site of HNgY in the solid. An example of a fruitful and enjoyable cooperation was a project in which the Helsinki group (Pettersson, Khriachtchev, Räsänen and others) prepared the new molecule HKrF in solid Kr, with support from calculations and modes by Zsolt Bihary and myself.

In 2001 it occurred to me that this family of molecules suggests by analogy a new and quite exciting organic chemistry of the noble gases. In cooperation with Jan Lundell, who visited, and with Arik Cohen, we predicted computationally the existence of HXeCCH and of HXeCCXeH, the first molecules made of noble gas atoms and hydrocarbon. Viewed as $(\text{H}-\text{Ng})^{+\delta}\ \text{Y}^{-\delta}$ type of molecules, the acetylenic group plays the role of the electronegative group. These predictions met with initial objection by referees, since the molecules were quite surprising and not noticed in previous experiments on acetylene in Xe. However, the paper was accepted in *J. Phys. Chem.*, and several months later, both HXeCCH and HXeCCXeH were obtained by the Helsinki group, and HXeCCH was produced independently by V.I. Feldman and his co-workers at Moscow State University. Shortly afterward, in cooperation with the Helsinki group (Khriachtchev, Lundell, Räsänen, and others) and also Arik Cohen and myself, HKrCCH was obtained and characterized. The discovery of the acetylenic noble-gas molecules seems to me quite important. First, in the few recent years since the discovery, several additional acetylenic compounds were obtained. The acetylenic bond clearly offers a range of new synthetic possibilities. Second, our calculations, mostly the work of postdocs Li Sheng and Eric Brown, predict the existence of extended species such as polymers and as molecular crystals (e.g., of HXeCCH). Third, calculations by Ehud Tsivion, a graduate student, show that HXeCCH is expected to be stable well above the cryogenic range, considerably above the presently expected stability range of other HNgY compounds. If compounds stable at room temperatures and above can be found, this may increase the prospects of practical applications for such materials. A recent noble-gas molecule prepared in Helsinki (Khriachtchev, Isokaski, and Räsänen) with support of calculations by Arik Cohen and me, is HXeOXeH, “di-xenon water”. This compound, I feel, may also prove of special importance in noble-gas chemistry. My fascination with new noble gas chemistry and with the surprises it offers continues. One direction we are currently exploring is the possible existence, not confirmed as yet, of noble gas molecules in nature, including both in terrestrial and in planetary environments. This is a very speculative but highly interesting and enjoyable search.

I would like to conclude this account by expressions of gratitude. I would like to express my deepest thanks to Anne McCoy, Anna Krylov, and Victoria Buch for editing this *Festschrift* for me. This is a very wonderful gift to me.

The outline of my career shows that I owe it mostly to the wonderful students and postdocs that I was fortunate to have. I am most grateful to my former and present groups. I have been very fortunate in having had very stimulating and inspiring collaborators, experimentalists, and theorists throughout my career. I benefited a lot from the collaborations and learned a great deal from them.

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