Autobiography of Michael L. Klein

I was born in London, U. K., on March 13, 1940, on City Road, which was within the sound of the bells of St. Mary-Le-Bow. My parents, Julius and Bessie (née Bloomberg) were both Londoners. Apart from brief periods, I remained in London during most of the Second World War. Not surprisingly, the London Blitz had a lasting impact on me. When I was young, the family moved frequently, eventually settling in Edgware, a North London suburb. My early experiences of school were unremarkable. I was blessed with an excellent memory and found arithmetic easy but much preferred to play football (soccer) than read or write. Homework was a problem, but fortunately my father hired a teacher to prepare me for the "eleven plus" grammar school entrance examination. This strategy evidently worked because in the fall of 1951 I attended the nearby Orange Hill Boys Grammar School, where I remained until I went to university. I immediately demonstrated an aptitude for mathematics and football and to a lesser extent track and field. As a teenager, a chance school visit to a holiday lecture by Lawrence Bragg at the Royal Institution greatly stimulated my interest in science.

Teenagers have a natural affiliation with pyrotechnics, and I was no different, being drawn to create impressive reconstructions of my early childhood experience of the London Blitz in school classrooms and the local park. At age 16, my father wanted me to join the family business. Luckily, I had a headmaster who could see beyond my exuberant youthful transgressions. Moreover, he was able to persuade my father that the study of science was a road to success and that I should be allowed to stay on at school and try for a State Scholarship to go to university. I responded to the challenge, and the final two years at grammar school were devoted to intense study of mathematics, physics, and chemistry in preparation for the arduous A-level and S-level examinations. As I recall, this was the toughest, most grueling period of my life—a month of exams set by Oxford *and* Cambridge universities, all passed with distinction. However, Oxford and Cambridge required Latin as part of their entrance requirements, so I looked elsewhere: London, Southampton, Exeter, and Bristol.

In 1958 I went "up" to Bristol University. There I became utterly seduced by a world of scholarship and learning. I finally enjoyed reading. How had I been able to make it to university without ever having read a novel? At Bristol I was exposed to enthusiastic and talented chemists, including Edward Abel, Alan Battersby, Douglas Everett, Noel Hush, Alan Leadbetter, David Ollis, and Wilson Baker, and physicists, including David Bohm, Peter Fowler, Charles Frank, Andrew Lang, Donald Perkins, Cecil Powell, and Maurice Pryce. These were heady days, and I became thoroughly enchanted on one hand by the beauty of natural synthesis (was this related to my passion for wine tasting?) and on the other by the elegance of theoretical physics. I would become an academic, but would it be chemistry or physics?

At Bristol, the final year included a research topic. Rumor had it that students doing synthesis were *required* to work weekends, so the dye was cast—I would do theory. Discussions with David Bohm's students Yakir Aharonov and Gideon Carmi and a seminar by Harold Friedman, who covered the blackboard with Greens functions, only reinforced this conviction. The department head Everett reluctantly allowed me to do theoretical research for my undergraduate thesis, even though he told me, "Chemists should wear a white lab coat." Noel Hush was on leave, so I was assigned to T. H. K. (Hugh) Barron—a theoretical physicist masquerading as a chemist (Hugh's D.Phil. was with Cyril Domb). So, in the summer of 1960, as a prelude to research, Hugh had me study books by Charles Coulson: *Valence* and *Electricity and Magnetism*. Everett decided that my undergraduate thesis should deal with ionic solvation, and this how I came to read the seminal papers of Bernal and Fowler and Pople on the structure of water. Little did I realize that this topic would recur time and again in my research! I worked diligently during my final year, in part because Cecil Powell had agreed to have me join his elementary particles group in physics for a Ph.D., provided that I obtained a "First" and a scholarship to fund myself.

As it turned out, I did manage to get a First Class Honors B.Sc. (1961) and a State Scholarship, but as lady luck would have it, the bureaucrats in London would not allow me to transfer my award for Ph.D. studies in chemistry to physics, even with the blessing of Everett and Powell. This is how I came to work with Hugh Barron for my Ph.D. Since there were no formal graduate lectures in chemistry, I was free to attend lectures in physics, which I enjoyed immensely. In all, I took Pryce's lecture in quantum mechanics 3 times! Being a graduate student was enormous fun, but living on the stipend was a challenge since about two-thirds was committed to rent. On June 3, 1962, I married Brenda May Woodman, who I had first met soon after arriving in Bristol. Our stable and mutually supportive relationship was a critical component in getting me through to the end of my Chemistry Ph.D. (*Thermal and Elastic Properties of Simple Lattices*, Bristol University, July 1964). Indeed, Brenda typed this hurriedly assembled thesis, which consisted of a few papers with their many equations and tables, on a portable machine in less than 1 week. Since carbon copies had to be made, the typing had to be essentially error free. The Barron and Klein papers dealing with the elastic behavior of solids under stress continue to be cited even today.

My first research paper was presented at the Low-Temperature Physics Conference (LT10) held in London in 1962. A group of the attendees, interested in rare gas solids, held an informal gathering at which I was approached with offers of two possible post-doctoral positions: one with George Horton's group at Rutgers (physics) was highly paid and the other with Giovanni Boato in physics at Genoa, Italy, came with essentially no stipend. As it turned out I was grateful for both offers. The challenge of finding funds to go to Italy led to my first research proposal and a fellowship from the CIBA Foundation. However, before going to Genoa, where I was to share an office with lifelong friend Giacinto Scoles, I spent a very productive summer in George Horton's group working on the theory of highly anharmonic solids. My daughter Paula was born in 1965, and I returned to Bristol as an ICI Fellow and joined the newly created Department of Theoretical Chemistry headed by David Buckingham.

In 1966 I again spent the summer working with George Horton and his group. Generous access to new IBM computers had allowed us to calculate the properties of rare gas crystals using the perturbation theory of Born and Huang. However, the second-order terms were surprisingly large, which caused

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us some concern. So, on returning to Bristol I wrote to Rudolph Peierls about this "problem". He immediately invited me to lunch at his college in Oxford and offered the following sage advice, "Young man, do not believe everything you read, no matter the author." I left with pointers to read about asymptotic series and Padé approximants. In 1967, discouraged by the job situation and computational resources, I left the U. K. with Brenda and Paula to once again join George Horton at Rutgers. This led to a very productive period working together with Victor Goldman on self-consistent phonon theory. However, I had now been a post-doc for 4 years, and it was time to look for a permanent job! There were a few tentative offers in the USA, but by far the most attractive was from Jim Morrison to set up a computational chemistry group at the National Research Council of Canada (NRCC).

Thus, my independent career began in November 1968 in Ottawa, where I stayed until moving to Penn in the summer of 1987. The 19 years in Canada were good. My daughter Rachel was born in 1969. Mentors, Jim Morrison, Fred Lossing, and Keith Ingold, not only allowed me freedom to pursue my own research but also regularly put me on outside assignment—most importantly to our sister organization (Centre Nationale de la Recherche Scientifique) in Paris. There I was free to collaborate with Jean-Pierre Hansen, Dom Levesque, Jean-Jacques Weis, and other visitors such as Ian McDonald in the burgeoning field of molecular simulation. These visits also enabled me to link up with the Centre Europeén de Calcul Atomique et Moléculaire (CECAM) (and hence Giovanni Ciccotti, Daan Frenkel, Jean-Paul Ryckaert and others), a productive relationship that continues to the present time. The NRCC also supported extended exchange visits with my contemporaries Ian McDonald and Jean-Pierre Hansen.

Life in a National Lab is essentially devoid of students. To compensate, through the 1970s, I taught summer school freshman physics at Rutgers—New Brunswick. I covered the whole year's syllabus in 12 four-hour evening sessions. Typically, I rented a house on the New Jersey shore and commuted to give the evening lectures three days per week. The rented house—better described as a shack—was a summer vacation home to not only my daughters Paula and Rachel but also to the children of relatives and friends. As it turned out the experience of dealing simultaneously with a freshman physics class and a group of teenage kids 60 miles away at the New Jersey shore taught me important management skills that have subsequently been put to good use in my present job. My co-conspirator on a few of these "adventures" was life-long friend and physicist Henry Glyde. During a typical evening the latest PRL was discussed over a shared bottle or two of California Cabernet and a barbequed two-pound steak while the kids busily graded the physics problem sets. It was during this time that I also became an Adjunct Professor of Physics at the University of Waterloo and Professor of Chemistry (part time) at McMaster University, a position I held for more than 10 years. Typically, I commuted to southern Ontario to teach during the winter semester, which gave some partial relief to the bitterly cold Ottawa winters. It is thus not an accident that I now live on the New Jersey shore.

In the 1980s, a diffcult time for research in Canada, my line manager Willem Siebrand fully supported my group and screened me from all administration. I was able to hire brilliant research associates such as Michiel Sprik and Shuichi Nosé, whose pioneering works on electron solvation with path integrals and simulation algorithms have stood the test of time. Roger Impey also played a critical role, being responsible for code development and bringing an informatics component to the group. This was the high point of my time at the NRCC, which included especially fruitful collaborations with David Chandler, Ian McDonald, and John Tse.

While my colleagues at the NRCC were very supportive, the overall situation of research in Canada was becoming miserable, even with the award of a Nobel Prize in Chemistry to John Polanyi. This fact, plus the urge to be embedded in a vibrant community of theoretical chemists (Hans Anderson, Bruce Berne, David Chandler, Bill Miller, Peter Rossky, Frank Stillinger, John Tully, and Peter Wolynes, to name just a few), and the prospect of garnering resources to tackle problems in the emerging field of molecular biophysics attracted me to Penn. I have not been disappointed. The collaborative environment at Penn has been truly outstanding. The move enabled me to not only initiate new fields of research and build on an enjoyable collaboration with Michele Parrinello but also to have a parallel career as director of the Laboratory for Research on the Structure of Matter.

Over the years I have been blessed with many talented and enthusiastic collaborators (far too many to mention here individually by name) that have shared my dreams and helped forge a common vision of computation as an enabling science and a true partner to experiment and theory. I dedicate this volume to them for their enthusiasm, hard work, and support. Without them my life as a scientist would certainly have been unfulfilled. This special issue is a truly wonderful birthday present and complement to the American Chemical Society symposium in San Diego and the Summer School in Erice, Italy. My gratitude goes to the organizers of these activities, especially to Ilja Siepmann, Doug Tobias, Mark Tuckerman, Robert Doerksen, Giovanni Ciccotti, Kurt Binder, and Mauro Ferrario. Finally, heartfelt thanks to David Chandler, Michele Parrinello, Michiel Sprik, and the minstrel David Coker for their cherished contributions.

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