Autobiography of Frank H. Stillinger

The factors that capture attention and create long-term interests in young children have been, and will remain, subjects of speculation and debate. This is certainly the case for those children who, as adults, eventually choose for their careers the highly focused professions of mathematics, engineering, and science. As a child of the Great Depression (born August 15, 1934) and of the Second World War, I have found it easy to believe that social stresses and values prevalent during those years must have exerted strong formative influences. In particular, the physical sciences at that time enjoyed a romantic aura that was propagated by newspapers and serious magazines, but that also was enhanced by the popular science fiction of that period that was offered in pulp magazines and low-budget movies. The notion that science could be the source of various dangers, such as nuclear threat and environmental insults, had not yet appeared. However, while this broad background without a doubt had a significant effect, in my own case, many specific memories seem to reveal that several other formative influences were also at play.

My earliest childhood was spent in the small New Jersey towns of Ewingville, Pennington, and Boonton. Vivid visual memories from that time—of huge lighter-than-air craft drifting slowly across the sky, likely on their way to, or from, Lakehurst, NJ—still remain. Those images seemed to have stirred a curiosity that later sought answers about how such floating behemoths could possibly work. Of course, this era soon terminated following the infamous Hindenberg tragedy on May 6, 1937.

That was also a time during which my parents, despite limited income, managed to expose their first child to a set of books revealing the wonders of the solar system astronomy and the age of dinosaurs. These engaging subjects quickly became the source of intense, almost mystical, flights of imagination. Certainly I was not the only child smitten by these topics at the time. A reasonable guess is that a large fraction of those from that era who, as I have, ended up in adulthood in the technical professions, would report similar childhood experiences.

The Second World War provided its own share of strong impressions. Gone were the dirigibles and autogyros of the 1930s, only to be replaced in the public eye with high-performance warplanes. I clearly remember these as a source of enthusiastic attention, at least by young males in grammar school. How were they designed? What was their horsepower? What top speeds could they exhibit? And what design characteristics allowed these aircraft innovations to appear?

During the early half of the 1940s, “Materials Science” had not yet been anointed as a distinct discipline. Nevertheless, the strategic importance of certain critical materials during those war years was very much in the public consciousness. Simple examples are often the ones that impress children the most. The one that I remember as especially noticeable by my schoolmates and myself involved the scarce national supply of copper. This was the traditional material of that backbone of the economy (as we perceived it!), the penny. Yet, for the year 1943, the United States found it necessary to convert the minting operation to producing zinc-clad steel pennies. Such a visually obvious modification could not help but create a lasting metallurgical lesson!

My high school education occurred in Scarsdale, NY, which was, at the time, and still remains, one of the wealthiest communities in the nation. My family, then including three younger brothers, inhabited the lowest income quartile locally, owing to my father’s modest income as a public school teacher of mathematics and industrial arts. This absence of disposable income at the time was a source of some personal discomfort. Scarsdale High School maintained high educational standards and was strongly committed to shipping a maximum percentage of its graduates off to college. Its mathematics and science teaching programs were certainly very good, but community standards and values seemingly placed primary emphasis on the business, medical, and legal professions. Consequently, the scientific encouragement available to interested and able students several miles to the south in technically oriented New York City high schools simply did not exist for me and my classmates. The relatively low percentage of the graduates who ultimately chose careers in technical fields reflected that distinction.

During junior high school and my early high school years, I must admit developing a strong antipathy toward the subject of English. Particularly annoying were the assigned readings of standard works in obsolete styles of writing, including poetry, drama, and novels. That antipathy inexorably translated into near-failing grades in those classes. However, a minor linguistic epiphany finally took place when I was a senior in high school. This occurred under the influence of an inspiring English instructor, perhaps because it was my first contact with a male instructor of that subject. The notion finally prevailed that language was a vital tool, even for scientists, and that communicating effectively and under a variety of circumstances involved skills that had to be learned and mastered. Flexible vocabulary, artfully chosen similes, unexpected humorous phrasings, and even creative sarcasm in the proper settings could be advantageous techniques.

High school graduation in 1951 was followed by four undergraduate years at the University of Rochester. This choice evidently was influenced by the fact that my mother had attended that university’s Eastman School of Music, as a voice and piano student. Chemistry was my choice of major there, following and focusing the developing interests of the preceding few years. It must be admitted that my decision to continue and expand in the scientific realm disappointed my mother to some extent. She had hoped to see a musical career emerge in her first child. However, that disappointment became somewhat mitigated as my three younger brothers showed greater affinities in that direction.

An obvious milestone encounter at the University of Rochester occurred during my junior year there (1953–1954). Professor Frank P. Buff was the undergraduate physical chemistry instructor then, and as a result of his lectures, I became strongly attracted to that area of chemistry, particularly as a budding theorist in statistical mechanics. During the following year, Frank Buff served as my senior advisor and mentor. My senior project involved theoretical modeling and numerical calculation of the surface tension for aqueous electrolytes. That work later generated my first scientific publication. This problem involved an alternative approach to one initiated by Lars Onsager and his student, N. N. T. Samaras, whose work was published in 1934 in Volume 2 of the *Journal of Chemical Physics*. An obvious consequence of that senior project was that I would learn about, and be inspired by, the remarkable contributions

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that Lars Onsager had made to statistical mechanics, one of which would later earn him the 1968 Nobel Prize in Chemistry.

Before joining the Chemistry Department faculty at Rochester, Frank Buff had earned his Ph.D. at Cal Tech under the direction of John G. Kirkwood. “Jack” Kirkwood had subsequently departed for Yale, becoming that Department’s Chairman, and also becoming an Onsager colleague there. Perhaps it was natural that I would be influenced to attend graduate school at Yale, and to consider one of these two giants of statistical mechanics as a Ph.D. advisor. The balance finally tipped in Kirkwood’s favor, in part owing to Onsager’s tendency toward mystifying modes of verbal communication. Over the years, this tendency had impelled graduate students in the department to confer an informal title on his statistical mechanics graduate course, “Norwegian I”.

My Ph.D. dissertation contained four distinct topics. Three were suggested by Jack Kirkwood: ion distributions in molten salts, the structure of electrical double layers at electrodes in concentrated salt solutions, and the partition functions for quantum fluids. The fourth was my own suggestion, to which Kirkwood seemed to take a liking. It amounted to a particle-size-coupling formalism for equilibrium distribution functions, some aspects of which were later developed by others under the popular title of “scaled particle theory”.

After receiving my Ph.D. in theoretical chemistry from Yale in 1958, another year was spent at Yale to allow my wife Dorothea to complete her Master’s Degree requirements in mathematics at the university.

During this additional year, I was classified as a Kirkwood postdoctoral collaborator, and under normal circumstances, it would have been a happy and productive time. However, Jack Kirkwood had developed a terminal case of cancer, which led to his untimely death at age 52 in August 1959. Watching the untimely demise of such an intellectually respected scholar is a sadly unforgettable experience.

A seemingly natural assumption held during the Yale years was that my professional future would be an academic career. But one result of the last few medically uncompromised discussions with Jack Kirkwood was that I also began to consider AT&T Bell Laboratories as at least a temporary alternative. By 1959, Bell Labs had earned a solid reputation as an excellent place to do basic research in the physical sciences. A logical strategy for a young person then was to spend a few years at such an institution, creating a significant publication record and establishing a respectable reputation, then transferring into academia at a somewhat advanced level. This would avoid the necessity of demeaning academic chores that reputedly were always dumped on junior faculty. As a result of such thinking, I joined the Research Area of Bell Labs in Murray Hill, NJ, in September 1959. The subsequent passage of time over many years witnessed a diminishing interest in the original plan to become an academic scientist. Whether or not it was a sensible judgment, my conclusion nevertheless was that whatever modest talents for science were present, they were not particularly applicable to effective teaching.

For approximately thirty years, the management at Murray Hill encouraged, and appropriately rewarded, its physical science researchers to pursue innovative basic and applied research. This was a nearly ideal setting for a young Ph.D. who was eager to set the intellectual world on fire, and there were dozens of us straining to do exactly that. Among other advantages that were present one would have to emphasize the low barriers between researchers from different academic disciplines. All of us were housed in the same interconnected building complex. Furthermore, it was an important aspect of the Bell Labs culture that one could freely walk down the hall to ask pertinent questions of a co-worker. Seminars were open to all and typically were attended by a broad spectrum of expertise.

As a result of the direct Kirkwood influence, and of interactions with many of his accomplished former students and co-authors, I had developed a strong research interest in liquid-state chemistry and physics. Pursuing that interest of course meant reading as many published papers on the subject as practicable and attending relevant conferences. Most notable among the latter was the biennial series of Gordon Conferences entitled “The Chemistry and Physics of Liquids”. All of these scientific interactions during the early 1960s produced a strange ambivalence. On one hand, the field exhibited an admirable level of erudition in the systematic and careful tradition that was the well-known Kirkwood style (but shared by many others). On the other hand, the status, style, and emphasis of the field produced an uncomfortable impatience. The fashionable liquid-state models that garnered most attention (hard spheres, Lennard-Jones “atoms”, etc.) were far too simple structurally to yield insights into the vast majority of real liquids that experimental science dealt with on a regular basis. Water was the pre-eminent and most obvious counterexample to the prevailing trend. This generated a personal decision to develop a systematic statistical mechanical formalism for water, both to stimulate deeper theoretical thinking about aqueous systems in solid and fluid phases, and also to induce the liquid-state community to tackle a wider spectrum of molecular substances and phenomena than it had been in the habit of examining.

The first phase of the water project got underway during 1967−1968, in collaboration with Arieh Ben-Naim, who was a postdoctoral associate. The principal objective was to construct an effective pair potential for water molecules that represented the formation of directional hydrogen bonds in at least a qualitatively correct fashion. This required considerable guessing, because rather little precise guidance was then available from direct quantum-mechanical computations for those interactions.

Molecular dynamics and Monte Carlo computer simulations had, by then, played a notable role in the physics and chemistry of simple liquids. Although computer power in the late 1960s was very weak by present-day standards, it nevertheless seemed to hold promise for penetrating the molecular mysteries of the water problem. A pre-eminent practitioner of the molecular dynamics variant of digital simulation during that period was Aneesur Rahman, who was working at the Argonne National Laboratory in Illinois. Both he and I happened to attend the Liquids Gordon Conference in August 1969, and as a result of conversations there, we agreed that the idea of a joint simulation project had substantial merit. Bell Labs was convinced to provide financial support to Argonne to cover most of the computer costs. The first of several joint papers that was co-authored with Rahman, covering a wide range of aqueous molecular attributes, appeared in 1971. Needless to say, computer simulations of aqueous systems presently continue to be a popular and vigorous research area, one outcome of which has been the appearance of vastly improved effective pair potentials, compared to the initial crude estimates of over 30 years ago.

The opportunities for other productive collaborations in the early years at Murray Hill were numerous and would require a much more extensive format than this to document in detail. However, it is important to mention one more notable example: Dr. Thomas A. Weber. Tom first joined Bell Labs at Murray Hill in a development group, but later successfully sought an internal transfer to my research area. He possessed formidable computer programming skills, complementing my almost-total computer illiteracy. We joined forces, and over a period of nearly 20 years, produced 42 publications.

Following the 1984 U.S. Justice Department's divestiture order for the Bell Telephone System, the previously encouraging environment for basic research began to change. These changes were almost imperceptible at first, but became increasingly intrusive. Lucent Technologies acquired control of Bell Labs at Murray Hill in 1996, and established its corporate headquarters there. It became increasingly clear to many of my colleagues in research there that their professional careers required moving to other institutions. By virtue of staying longer at Murray Hill than many others did, I experienced an involuntarily transfer to a Lucent spinoff, Agere Systems, which had an even more impatient attitude toward basic research. My employment there terminated in June 2001.

Toward the end of 1996, I was invited to be a frequent visitor at Princeton University, for purposes of scientific collaboration with Professor Pablo G. Debenedetti and his group of students. This provided a welcome contrast to the other situation 30 miles to the northeast and generated several engaging research projects. The Princeton connection has subsequently expanded to include the Chemistry Department, thanks to Professor Salvatore Torquato, with whom other collaborative research projects have also been productively pursued. The Princeton connection continues at the time of this writing.

Autobiographies are intrinsically unfinished stories. Those of us who inhabit the world of scientific research continue to marvel at the unanticipated directions in which its advances take us. It remains to be seen what additional chapters the present story will eventually require.

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