

Kuppermann, 1996 Photo ID 96-188A

ARON KUPPERMANN
(1926 – 2011)

INTERVIEWED BY
SHIRLEY K. COHEN

**July 17 and 24, September 13 and 25,
and November 15, 2001**

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CALIFORNIA INSTITUTE OF TECHNOLOGY
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Subject area

Chemistry, chemical physics

Abstract

Interview in five sessions (July-November 2001) with Aron Kuppermann, professor of chemistry, Caltech. Kuppermann, born in São Paulo, Brazil, discusses his family, childhood in New York City and São Paulo, and education. Degree in chemical engineering in 1948 and in civil engineering in 1952 from Escola Politecnica at the University of São Paulo. Joins faculty at Instituto Tecnológico de Aeronáutica in São José dos Campos. Takes physics classes and first course in quantum mechanics with David Bohm. Marries Roza. Fellowship for study in theoretical chemistry and radiochemistry at the University of Edinburgh (1953), followed by graduate work at University of Notre Dame (with Milton Burton); PhD, 1955. Hired as assistant professor of chemistry at University of Illinois, Urbana; research into measuring triplet states of molecules; unimolecular decomposition processes; use of digital computer ILLIAC 1; calculating electronic properties of molecules (with Martin Karplus). Joins Caltech faculty in physical chemistry, 1963.

At Caltech oversees installation of new molecular beam machine brought from Illinois. Discussion of construction of Arthur Amos Noyes Laboratory for Chemical Physics and the chemistry division faculty from his early years: W.

Robinson, H. Gray, J. H. Sturdivant, S. Chan, R. Badger, R. Pitzer, W. Goddard and B. V. McKoy. First classes in undergraduate physical chemistry and graduate course in statistical mechanics. First sabbatical (1968) spent at Weizmann Institute in Israel and FOM Institute for Atomic and Molecular Physics in Amsterdam. Upon return, research focused on quantum mechanical theory of chemical reactions. Granted use of big computer at Ambassador College with George Schatz. Experiments in electron scattering and mono-energetic reactions photoelectron spectroscopy. Interest develops in a more theoretical approach to problem solving.

Discusses extensive committee work and civic interests. Discusses involvement in joint American-Brazilian program, started by Carl Djerassi of Stanford, to encourage chemistry research in Brazil (1969-77). Consultant to World Bank loan projects for scientific laboratories in Brazil and, later, China and Mexico. Guest professor at Shandong University (1984). Executive board member of National Partnership for Advanced Computational Infrastructure. Thirty-year involvement with Villa Esperanza, after daughter Sharon was born with Down syndrome. Talks about sociological changes at the institute. Students who are leaders in the field of quantum reaction dynamics: D. Truhlar, G. Schatz, and J. Bowman; plus J. Kaye at NASA. Philosophy about sabbaticals in aiding his scientific activity.

Administrative information

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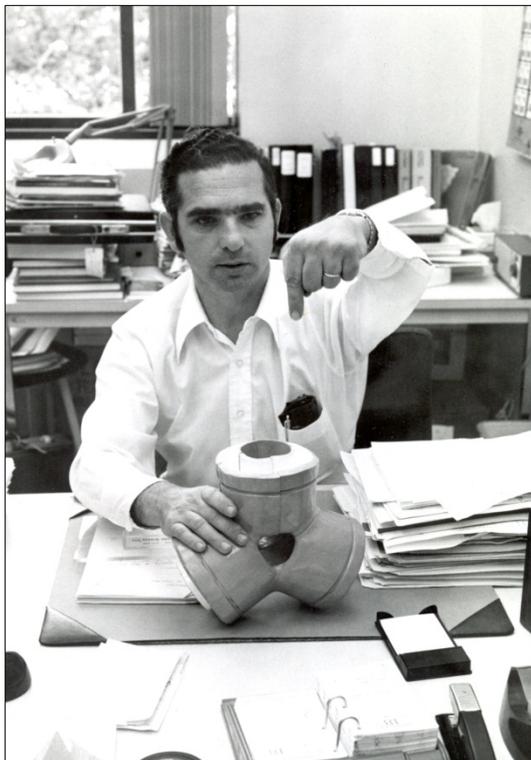
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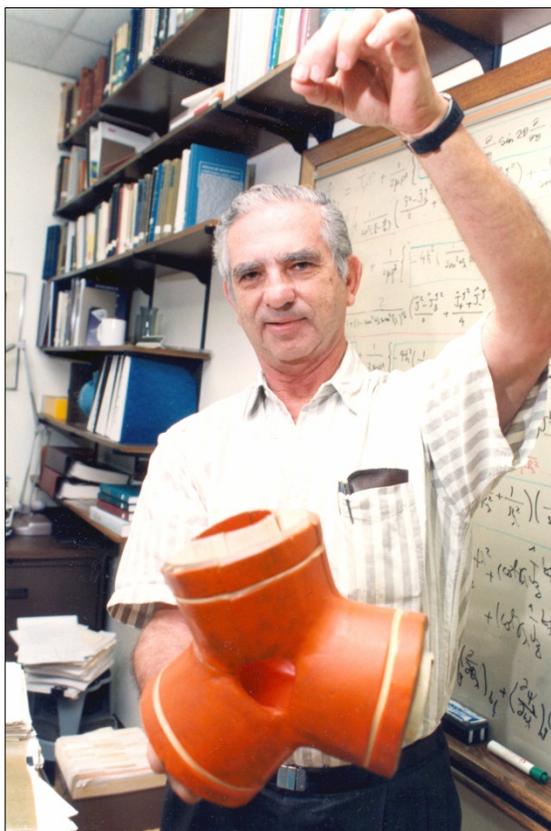
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Kuppermann in 1973 with his balsa wood model—conceived, designed, and built by Kuppermann—illustrating the potential energy in a chemical reaction. Photo ID 74-80-2-32



Kuppermann in 1996
Photo ID 96-188A

CALIFORNIA INSTITUTE OF TECHNOLOGY ARCHIVES

ORAL HISTORY PROJECT

INTERVIEW WITH ARON KUPPERMANN

BY SHIRLEY K. COHEN

PASADENA, CALIFORNIA

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INTERVIEW WITH ARON KUPPERMANN

Session 1

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Family roots in the Ukraine and Poland; born in São Paulo, Brazil; family moved to New York; moved back to Brazil with father at age 6. Obtained a degree in chemical engineering at the University of São Paulo; joined the faculty of the Instituto Tecnológico de Aeronáutica in São José dos Campos. Interest in chemical bonding led to study of quantum mechanics with David Bohm at the University of São Paulo. Met wife Roza when she was studying chemistry at the University of São Paulo.

In 1953 received fellowships to study radiation chemistry first at the University of Edinburgh and then at University of Notre Dame, with a summer course in radiochemistry at Harrow, England. In 1955 obtained a PhD in Physical Chemistry at Notre Dame; accepted a chemistry instructor position at the University of Illinois along with Martin Karplus, Bob Rubin, and Rolfe Herber; had to return to Brazil to change visa status.

Session 2

22-40

Explanation of a triplet state; discussion of the work of Sir Cyril Hinshelwood and Nikolay Semenov. Designed and built an electron scattering apparatus at University of Illinois; tested Hinshelwood's unimolecular decomposition hypothesis; used a digital computer to understand radiation chemistry. Description of the development of the electronic digital computer; use of ILLIAC 1 to solve equations used in John Magee's theory with methodology developed by John Todd. Collaborated on research in quantum chemistry with Martin Karplus. University of Illinois graduate students included Lionel Raff and John G. Larson.

Description of development of classical trajectory equations by Henry Eyring and Joe Hirschfelder at Princeton using an electromechanical Marchant Machine; Jerry Hiller and Jacob Mazur resumed that work using ILLIAC 1; Hiller composed the "ILLIAC Suite" on ILLIAC 1; Karplus continued that work at Columbia University and developed CHARMM.

Summary of projects at University of Illinois. Decision to leave University of Illinois. Spent a year in Brazil in 1960, but decided against staying. Declined offers from Indiana University and Columbia University. Wilse Robinson and Hardin McConnell recommended Caltech make an offer; accepted and came in 1963.

Session 3

41-62

Arrived at Caltech August 1963. Remodeled laboratories in basement of old Gates building; participated in design of laboratory in the new Noyes building; moved into Noyes in 1966.

Chemistry division at Caltech in 1963 included Wilse Robinson, Sunny Chan, Hardin McConnell, and Russell Pitzer. Bill Goddard, Vince McKoy, and Rudy Marcus joined later. Happy with the high quality of Caltech students and the machine shop. Began teaching in the two courses: undergraduate physical chemistry and graduate statistical mechanics. Family happy with the move to Pasadena. Took first sabbatical leave in 1968, spending the first half at the Weizmann Institute of Science in Israel, and the second half at the FOM Institute for Atomic and Molecular Physics in Amsterdam. Began research on the quantum mechanical theory of chemical reactions; given access to computer at Ambassador College; research expanded from three atoms to four atoms and to larger molecules.

Caltech committee work included serving as chair of committee for relations with the community set up by Harold Brown. Served on committee appointed by Judge Manuel Real to make recommendations about segregation in Pasadena schools. Appointed by Murph Goldberger to a committee to look into Caltech's computing needs; still a member of the computing advisory committee. Disappointed that Caltech never got a commercial vector computer and that its parallel computing activities are not the best.

Session 4

63-85

In 1968 began involvement with program started by Carl Djerassi to help modernize chemistry in Brazil. Fred Johnson, Harry Gray, George Hammond, and Charlie Overberger also participated. Hired as a consultant in 1983 to review World Bank loans to support and improve science in Brazil; description of World Bank program in Brazil. Taught modern quantum reaction dynamics at Shandong University in China in 1984 as part of a World Bank program. In 1989 asked by Barbara Searle to advise on second World Bank loan to China. Consulted on a World Bank program in Mexico. Currently a member of the executive board of the National partnership for Advanced Computational Infrastructure working on distributed teraflop initiative.

Came to Caltech when Lee DuBridge was president and Arnold Beckman was chairman of board of trustees. Harold Brown was a good administrator, while Murph Goldberger was a people person. Parallel computing flourished under Goldberger but received less funding under Thomas Everhart; Everhart was too cautious. Thinks David Baltimore is not putting enough funding into the Center for Advanced Computing Research.

Session 5

86-99

Involvement in Pasadena community began with founding the Housing Information Service in 1965; member of the Pasadena Educational Foundation; member of the board of directors of Villa Esperanza, a program for children with Down syndrome.

Three ex-graduate students are leaders in the field of quantum reaction dynamics: Don Truhlar, George Schatz, and Joel Bowman. Jack Kaye is with NASA.

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Interview with Aron Kuppermann
Pasadena, California

by Shirley K. Cohen

Session 1	July 17, 2001
Session 2	July 24, 2001
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Begin Tape 1, Side 1

COHEN: Good afternoon, Professor Kuppermann. This is July 17, 2001. We are delighted that you're going to participate in this project. A good place to start is to tell me something about your family and how you came to be.

KUPPERMANN: Certainly. I'll start with my mother. She was born in the last century, about 1898, in a small village in the Ukraine by the name of Trostianets, which is about 150 miles, roughly speaking, southwest of Kiev. At the age of fourteen, she accompanied four older half-brothers in their immigration to the United States. It was a first step of the family move. She left behind a full brother and sister—a pair of twins—and her mother. They—her mother and the sister and brother—immigrated to Brazil, probably in the early 1920s. When my mother became an American citizen and was an adult, she decided to go to Brazil to visit her mother, whom she had not seen for about ten years. In São Paulo, Brazil she met my father. He was born in Warsaw, Poland at about the same time that she was. He left home at the age of eighteen and spent four years or so in Germany, where our last name got its Ps and Ns doubled. He moved to Brazil in 1922, and met my mother in São Paulo in 1924. They married, and I was born in 1926 in São Paulo.

COHEN: What language did they have? Your mother would hardly have known Portuguese.

KUPPERMANN: Yiddish. Yiddish was the home language both for my father and for my mother. They communicated in Yiddish forever. That was always their common language.

About six months after I was born, my mother became unhappy with living in São Paulo, Brazil. That was a very provincial, small town for her standards, having spent her teenage and early adult years in New York. She convinced my father to move to New York, and at that age I became a US resident.

COHEN: But you were born in Brazil.

KUPPERMANN: I was born in Brazil, right. When I was about three years old, my mother came down with breast cancer, and she was hospitalized for about three years, during which I lived in a variety of foster homes and orphanages. Those were the Depression years, and my father had to earn a living, so he could not keep me at home.

COHEN: There was no other family that could take you?

KUPPERMANN: No. He had a sister in New York, and my mother had brothers in New York, but they were all under Depression pressure and, for whatever reason, were unable to take me in. She died when I was about six years old. At that time my father decided that the best thing would be for him to return with me to Brazil, where the battle for a living was less intense, and he could live with me, which indeed was the case. He rented a room in a family home in Santos, Brazil, not quite São Paulo. During the day I went to school. He dropped me off and picked me up every day.

COHEN: He was a single parent.

KUPPERMANN: He was a single parent, that's right. That was in about 1933-34. My very early schooling was at a private elementary school in Santos called the Anglo-American College, which catered mainly to diplomatic families from English- and otherwise-speaking countries. I spent about two or three years there before he remarried and moved to São Paulo.

COHEN: Did he want you to have English as a language?

KUPPERMANN: Yeah. He wanted to keep the English up. The school taught in Portuguese, not in English; nevertheless, a large number of the families were English-speaking families. He spoke with me in English. He wanted to keep the language up.

When I was about ten or eleven years old, he remarried a widow. They had no other children so I grew up as an only child in São Paulo, where I finished my elementary school in another English-catering school, called Stafford College. Then I went to high school in a private school.

COHEN: Your father must have made a reasonably good income to send you to a private school.

KUPPERMANN: It was a very high priority for him. He had a small haberdashery, and that was barely enough to eke out a living. We didn't really have a home for the first two or three years in São Paulo. He had a little haberdashery store. The back of the store had a room where my stepmother cooked the meals and where we spent the days as if it were our home. Then we went at night to a pair of rooms rented in the home of a Jewish family in São Paulo. My father and stepmother had a small bedroom downstairs and I had a small bedroom upstairs, but we only slept there; we had no meals there. That went on for about two or three years until the situation was financially stable enough for them to rent a house. That is the house that I lived in from the age of about twelve until I got married—until age twenty-one—except for a few years when I was teaching at a university outside of São Paulo, where I had my own house. I was married to Roza by then, so indeed I lived from twelve to twenty-one at that nice little house in São Paulo.

COHEN: And you went to school there.

KUPPERMANN: Yes, I went to school there, at a high school called *Gymnasio Osvaldo Cruz*. *Osvaldo Cruz* was a famous Brazilian diplomat, and this was a private high school named after him. It was a five-year high school in those years, after which I took an examination to enter what they called pre-university. The University of São Paulo was really not a university in the American sense but was a collection of independent schools and departments. The one I went to

was the engineering school, called Escola Politecnica, which was patterned and founded after the French Ecole Polytechnique, except that it had no military association.

COHEN: Was this officially still high school years?

KUPPERMANN: It was neither high school nor university. What they called it in Portuguese was pre-university. There was an entrance examination, a fairly rigorous one, so the admissions rate was relatively low. Then it took two years, which would have been the sixth and seventh year of high school, so it would have been the eleventh and twelfth years of an American high school because the elementary school was five years long.

COHEN: It was hard to get into, because it was by examination.

KUPPERMANN: That's right.

COHEN: But it was a government school, right?

KUPPERMANN: It was a government school.

COHEN: You didn't pay to go to that school.

KUPPERMANN: No, that one was free—the first free school I had. Then, after the two years, you had to take another entrance examination from the pre-university to the university. It wasn't required that you take the two years of pre-university at that school. You could have done that elsewhere. But everybody then had to take an even more restrictive examination to enter the engineering school. It wasn't the university; it was the engineering school. People entering chemistry took an examination in the chemistry department of the faculty of sciences, and the physicists took a separate one. Each department, each faculty of the university, had its own entrance examination. This was a fairly tough one. The ratio of candidates to acceptances, if I remember correctly, was something around five to one. To the chagrin of my father, I entered in second place. I didn't get the first one, for the reason that those years really were very upsetting to me. Among the entrance topics, there was one on sociology. The sociology exam had two

parts: the first part was an essay, and the second part was a large number of questions. That essay was mentioned in the first line in small letters, and I simply didn't notice it, so I simply left the essay blank. It was a relatively simple topic, on what social facts are, or something of that nature, and it went blank, and that cost me a major chunk of grade. Otherwise, I probably would have—

COHEN: So you were still second.

KUPPERMANN: I was still second.

COHEN: You must have done very well on the other part.

KUPPERMANN: Anyhow, I worked very hard. The engineering school was patterned after the European schools and the Ecole Polytechnique. We had, roughly speaking, forty-eight classroom plus laboratory hours per week on the site, in addition to whatever homework and studying needed to be done. In other words, it was six days a week and eight hours a day of classroom and laboratory instruction. I graduated from there as a chemical engineer.

COHEN: Did you enjoy it though?

KUPPERMANN: Yeah, I enjoyed it.

COHEN: Was this all boys, or were there girls in this school, too?

KUPPERMANN: It was not restricted, but in the whole engineering school the number of girls who were my colleagues was two or three. Sociologically, girls did not have an interest in engineering.

COHEN: Which continues. [Laughter]

KUPPERMANN: In any event, I did very well. I got a couple of medals, one in calculus and one for graduating as the best chemical engineering student. The main issue then was what to do

afterwards. My original plan had been to try to find a job as a chemical engineer, but in my last year there, a new university, or aeronautical engineering school, opened up under the auspices of the Brazilian air force, in a town that was about a hundred miles away, São José dos Campos. The Brazilian air force had decided that they didn't have any native-trained people to design and build airports, and that the aircraft that they could buy were not appropriate for Brazilian conditions in the boondocks, where you needed short landing strips and aircraft that could take off and land on small pieces of land.

COHEN: Did this have anything to do with the Second World War? I mean, Brazil was not in this war.

KUPPERMANN: No, it was. Brazil entered late in World War II and did send troops to Italy. It also was used as an important American base. The northeast of Brazil, particularly a city—the capital of the state Rio Grande do Norte was Natal—and the distance between Natal, in that bulge of Brazil, and Dakar, in Africa, was the shortest distance across the Atlantic.

COHEN: Plate tectonics.

KUPPERMANN: That's right, exactly. During World War II, when the submarine warfare was intense and relatively few American ships got through—many of them were sunk—this other route by planes—just ordinary aircraft with propellers—the maximum range they had was exactly the distance from Natal to Dakar. That became an extremely important traversal part and means of transporting troops and a certain amount of goods from the US to the European theater. So there was a strong American presence in the north. Eventually Brazil entered the war towards the end, sending troops when the US was already invading Europe through Italy. So there were Brazilian troops in the war.

COHEN: But this sounds like they were not very effective in that war.

KUPPERMANN: No, not really, other than rationing. Brazil didn't have at that time a native oil industry and hence all gasoline it consumed was imported, and there was none of that. So they developed these carbon monoxide fuels. Big, vertical tanks, like heating tanks, were powered by

wood in the back of the car. The carbon monoxide that they gave out was injected into the ordinary gasoline engine and was consumed in lieu of gasoline.

COHEN: And it worked?

KUPPERMANN: It worked.

COHEN: People survived?

KUPPERMANN: That's right. It was amazing how ingenuity was good enough to allow them to have a certain number of those—it wasn't that most families had a car propelled that way, but there were a few.

COHEN: Did you go to this aeronautical engineering school?

KUPPERMANN: The Brazilian air force wanted to create a high-powered engineering school for aeronautical engineering and closely related forms of engineering—mechanical engineering, metallurgical engineering, airport engineering, and aircraft engineering—so they went to MIT to get somebody to help them out. There was a retired dean of the engineering school, a man by the name of Smith—that's not very helpful; I don't remember his first name—who agreed to come down to Brazil and create from scratch this school, which he did, and it still exists. [Instituto Tecnológico de Aeronáutica established by Richard Harbert Smith *-Ed.*] At one time it was considered the best engineering school in Brazil. I was on the faculty of the opening group. There was a chemical engineer who was an assistant professor at the polytechnic school. I was a student in a class he taught, and he invited me to go to—

COHEN: And this was without any advanced degrees or anything?

KUPPERMANN: No. Advanced degrees, especially in engineering, were an unknown type of institution. Even in the sciences, the number of people who had PhDs could be counted on almost all of the fingers of a small number of hands. So graduate school was, essentially, for all practical purposes, an unknown institution at the University of São Paulo, which was the best university in the country. So I just started. However, in the process of studying engineering, I

started becoming very interested in science. I went into chemical engineering as something that might permit me to earn a living, but I really was curious about science. Once, while taking an organic chemistry course, I asked the professor, who was an elderly old-fashioned man, how a certain chemical reaction took place in a double-bonded molecule where, when you added hydrogen chloride, the double bond connected the last carbon atom on propylene or glutamine to the next. The carbon added with the chlorine, not on the end atom, but on the next-to-the-end atom—not the other way around—even though it's a double bond and one would expect it to be the other way. That was known for a century; it was called Markovnikov's Rule. I asked him why that was so, and he said, "Oh, don't ask silly questions. That's the way nature is."

COHEN: I see. This was science at that time.

KUPPERMANN: That's right. It was organic chemistry in an engineering school. I was still curious, so I went to see my physical chemistry professor. He was a very practical empirical guy and he didn't know either, so I went to see his assistant professor. The structure was Germanic in style, so that assistant professors were under a professor—invited and fired by them. I went to the assistant professor, and he was a younger and more interesting man. His name was Fausto Walter de Lima. He is still alive and I still interact with him. He told me, "I really don't know the answer, but I just saw a book with a title that may be related to it." The book is called *Valence*, in English, and the author was Coulson. Coulson was a world-class theoretical chemist at Oxford who wrote this book to make quantum mechanics as applied to understanding chemical binding more accessible to the general scientific population. This was still early in the game. Chemists didn't know any quantum mechanics. Charles Coulson himself was a mathematician by training and got into chemistry through quantum mechanics and mathematics. I got that book, and the fact that I was able to read English was very helpful.

COHEN: I was just going to say it must have been in English.

KUPPERMANN: That's right. I read it, and it was all qualitative—there were essentially no equations—with words like "the way function represents the probability of finding a particle someplace or other—" It didn't make sense to me, but there was a reference in it to a book by [Henry] Eyring, [John] Walter and [George] Kimball. Henry Eyring was a very well known

professor, a chemist who introduced the theory of absolute reaction rates while he was at Princeton. Together with Walter and Kimball he wrote this book called *Quantum Chemistry*, published circa 1945. So I went there, and it was full of equations. It was so full of equations that it was beyond my training in physics, because the engineering school in physics was purely classical physics, and the calculus was purely first- and second-year current calculus. Quantum mechanics involves partial differential equations, and I had never seen those. I knew that that area of knowledge was what was going to have the answers to my curiosity-driven questions. I decided I had to go and get a degree in physics in order to be able to learn the fundamentals that would permit me to learn quantum mechanics. So I took another entrance examination. Although I was in my last year of chemical engineering, I had to take another entrance examination in the physics department to be admitted—not the physics department at the engineering school, but the physics department of the school of science and letters. I had to take freshman calculus—everything that I had already taken.

COHEN: So in a sense you were starting again.

KUPPERMANN: I had to start again. That was the only way. While I was in my last year or two of chemical engineering, I also doubled and officially took these courses, cutting most of them and showing up for exams. It was all material I knew. When I finished the second year, I graduated from the engineering school and moved to this Instituto Tecnológico de Aeronáutica, the Aeronautical Technological Institute.

COHEN: All this good Portuguese we have here.

KUPPERMANN: Yes. So I was working full time there. I moved and had a little house there. Roza and I got married just before that, so she was still studying chemistry at the university.

COHEN: You met her at the university?

KUPPERMANN: No. [Laughter] I'll be glad to tell you how I met her, but let me just finish the thread and then I'll go back to that.

I was spending my weeks at São José dos Campos. I would go there Sunday night, to be available for Monday classes, building laboratories, and so on, and then I would come back on Saturday afternoon. So I really was not able to attend the third-year physics courses. Nevertheless, I took those courses by reading myself. It was in that period, maybe just before I moved to this new university, that I took my first course in quantum mechanics with a man by the name of David Bohm. David Bohm was a then famous—now infamous—young American physicist who had gotten his degree with [J. Robert] Oppenheimer and then joined the faculty at Princeton. It was then that he was called by the House Un-American Activities Committee to testify about his involvement with Oppenheimer and with Communists. He refused to answer any questions about anybody other than himself. He was open and frank and said, yes, he was not a Communist, but he was very sympathetic and he had many Communist friends. When they started asking him who they were and what they did, he refused to answer. He was within his legal rights, and so he was not declared in contempt of Congress, but he became notorious. He was an assistant professor at Princeton, and towards the end of his third year they decided not to renew his appointment, even though he was very, very promising. He published at that time a superb book on quantum mechanics that, even though it was published in 1951 or '52, is still currently used by many people, including myself. He had to find a job in a hurry, and he found one in São Paulo. That was exactly when I was entering my third year in the physics department and took his quantum mechanics course.

COHEN: He came because there was nothing in this country available to him?

KUPPERMANN: Yes, even though he was brilliant. He was extremely promising. He did wind up having a distinguished although controversial career, because he invented a new interpretation of quantum mechanics that was different from the Copenhagen probabilistic one. It was a deterministic one, and it was really frowned upon over the years—except that more recently it has become less rejected and more in vogue. There are many, many people using that way of looking at quantum mechanics, myself included. I've been using this perspective to find out how chemical reactions occur, and I have a much greater insight, because it permits you to think classically without using an approximation. It shows the equivalence of classical and quantum mechanics. For him, quantum mechanics is identical to classical mechanics but there is an

additional force of nature, which he calls the quantum force, which, when injected into the classical equations, or most Newton equations, makes them become Schrödinger equations. So it is exactly correct. There is no difficulty with the mathematics. The difficulty is with the philosophy or the interpretation—the words that you attach to the meaning of the quantities that appear in the equations. That is where all of the controversy is, and that is what is slowly changing over time. Anyhow, this was a wonderful opportunity for me to learn quantum mechanics. It strengthened my curiosity and my desire to reach what were the frontiers of knowledge at the time, which I was starting to get an inkling of.

COHEN: So that was just luck in some ways.

KUPPERMANN: Sheer luck. It was driven by my initial curiosity of going from why that chemical reaction occurred that way to taking a degree in physics and, through that, meeting Bohm accidentally.

COHEN: Did he stay in Brazil after all the politics was over?

KUPPERMANN: Yes, but he never came back to the United States. I believe—I'm not sure—that his passport was taken away from him, although he was an American-born citizen. After a couple of years in Brazil he went to Israel—to Haifa, to the Technion. I'm not even sure he's Jewish; his background is Pennsylvania Dutch. From there, he finally found a position in Bristol, where he was a professor of physics for a significant number of years. Then he moved to Birkbeck College, London, where he spent the last twenty years of his career as a professor of physics, fundamentally focusing his attention and expounding on his reinterpretation of—

COHEN: So this man really had a profound influence on your life in many ways.

KUPPERMANN: Not a continuous one. There was this original one in which I first really learned quantum mechanics from him and acquired a curiosity about his reinterpretation of quantum mechanics. When I came to the United States about two years later as a first-year graduate student, I had to give a seminar, and I picked Bohm's reinterpretation of quantum mechanics as my topic. I was at Notre Dame then. In preparation for that seminar, I wrote to all who I

considered to be the outstanding theoretical physicists in the world, namely [Albert] Einstein, [Richard] Feynman, [Werner] Heisenberg, [Arnold] Sommerfeld, [Leonard] Schiff. Schiff had written a book on quantum mechanics. He wasn't really in the same class as the others, but for me—I didn't know any better—anybody who writes an important textbook must be—and I got answers from many of these people. Einstein wrote back a wonderful letter discussing why, although he was in great sympathy with Bohm's idea, because it was more deterministic and along the lines of God not playing dice with the universe, it turns out—I didn't know it from his letter, and only found out much later—it turns out that Bohm, while at Princeton, had discussed his reinterpretation ideas in great detail with Einstein. So Einstein was very well versed on it, and maybe that was the reason that he found it appropriate and not too difficult to write me a two-and-a-half-page letter saying in detail why, although he was sympathetic, he didn't agree with it. Most of his reasons went down the drain, and were found not to be appropriate over the years. I still have that letter.

COHEN: I was going to ask you if you still had the letter.

KUPPERMANN: Yes. Judy Goodstein has a copy of it. This came up ten or fifteen years ago, and she asked for a copy and I gave it to her. It was very, very interesting. His objections were important objections, but science overtook them. He was unhappy that it would make quantum mechanics be what you'd call non-local, that you'd have instant communication at a distance. Well, that's exactly what has been proven to be the nature of nature with these experiments in France—[Alain] Aspect and so on—done about fifteen years ago [reference is to Alain Aspect's Bell test experiments done in the 1980s in connection with Bohm's idea of hidden variables. — Ed.]. It's the nature of the world. You may not like that kind of world, but that's the way the world is, so to use that as an objection to the reinterpretation was not a valid objection, because the reinterpretation isn't what brought about that non-locality. It was the experiments that gave non-local—. Anyhow, that's getting off on a tangent.

COHEN: We ought to go back to where you were. You've jumped to the United States, but you're still doing physics with Bohm. That's where we left off.

KUPPERMANN: Well, I didn't do any physics with Bohm. I just took a course with him. After I gave this seminar at Notre Dame, even the most sympathetic guy, Einstein, said that he couldn't agree with it, so I dropped that. I didn't pursue that after this wonderful series of letters, and I went into different things.

But you were asking about Roza. I met my wife, Roza—she was studying to take the entrance examinations to the chemistry department of the school of sciences at the University of São Paulo. People took cram courses to pass those exams. To help earn a living—my parents were of very modest means—I taught one of those cram courses, and she was a student in one of them. That's how we met; she was a cram course student of mine. We had just been married when I moved to this aeronautical engineering school, and she was still living with her parents, finishing up her last year of chemistry in São Paulo while I was in São José dos Campos.

COHEN: So then you finished your university degrees.

KUPPERMANN: I had finished the chemical engineering degree. I had not finished, and never did finish, the physics degree. It was looking more and more like it was hard to earn a living as a chemical engineer in São Paulo. You had to be an employee, and the salaries of employees, even technically skilled people, were not sufficient to earn a reasonable standard. I also reentered the university's engineering school and was working on a degree in civil engineering, because civil engineers were starting to become very prominent. They became contractors, and several of my friends and relatives—

COHEN: Ah, so this was just the nature of earning a living.

KUPPERMANN: That's right. To earn a living, I started taking this civil engineering degree while I was teaching in São José dos Campos, and I was married. Then I decided I really needed to learn more science. I applied for two fellowships abroad, one in the United States through the Institute of International Education, and the other in Britain through the British Council.

COHEN: So it wasn't to a specific school.

KUPPERMANN: Well, in one case it was, and in the other it wasn't. The British Consulate had a thick book describing all the universities in Britain and the courses they offered. It was almost like a catalog, but rather than a single university, it was a "Reader's Digest" of all the British university catalogs. I was interested in two things: theoretical chemistry and quantum mechanics. I also needed to get back to Brazil and earn a living. They had a new institute for atomic energy with a new nuclear reactor that had just been put into operation. I thought that if I studied radiochemistry, I could find a position there while still being able to pursue my real interest. So I went down the list and I found one place only in Britain where I could study both what I thought was radiochemistry and also theoretical physics, and that was in Edinburgh.

COHEN: Which isn't even in England; that's Scotland.

KUPPERMANN: That's Scotland. That's right. Max Born was in Edinburgh, and that would have been a very—

COHEN: Another refugee.

KUPPERMANN: That's right, another refugee—and there was a man doing what turned out to be radiation chemistry, which is not radiochemistry. It's very different from radiochemistry. In my mind, I didn't know the difference. I had never come across the words radiation chemistry, and I just thought it was the British vernacular for radiochemistry. Radiochemistry is the chemistry of radioactive isotopes.

COHEN: I see. I didn't know that.

KUPPERMANN: Radiation chemistry is the effect of ionizing radiation, like gamma rays, alpha particles, and so on, on molecules. It has nothing to do with nuclei; it has to do with ordinary chemistry. As a result, they are totally different fields—unbeknownst to myself. So I applied specifically to Edinburgh—well, through the British Council to go to Edinburgh—and the British Council gave me a scholarship to go to Edinburgh and do those two things.

COHEN: What year would that have been?

KUPPERMANN: 1953. I also applied to the Institute of International Education, which was under the auspices of the US Information Agency, to go to graduate school in the United States. There you didn't apply to a specific school. I just made a list. I told them I wanted to study theoretical chemistry and radiochemistry, and here was my list of preferences: number one, Caltech; number two, Berkeley; number three, Harvard; and I don't remember four and five. What I got back from them eventually was a letter saying that the University of Notre Dame was pleased to offer me a scholarship. I hadn't the foggiest idea where the University of Notre Dame was. As a matter of fact, when I first saw it, I thought that somehow they had a connection with France and this was some university in France. Years later, Linus Pauling told me what happened. This was an incredible fluke, an accident. I was here at Caltech already by then. In a conversation this story came up, and I said, "Many years ago I was interested in coming to Caltech as a graduate student, but I didn't get any offer from Caltech. I didn't apply to Caltech directly, either." Pauling said, "Oh, I remember that. I was chairman, and I remember your papers. These papers from a Brazilian came up, and he wanted to study theoretical chemistry and radiochemistry. I said, 'Well, certainly we have theoretical chemistry at Caltech, but we have no radiochemistry.'" He remembered there was a Faraday Society meeting not too long ago at which he met two people from Notre Dame, one of whom was a theoretical chemist who he then got to know, John Magee, and the other was a radio chemist, Milton Burton. So he thought, "Notre Dame has them both," and he wrote back to the Institute of International Education saying that Caltech didn't have what this young man wanted but Notre Dame did. It turns out that he was mistaken. He confused radiochemistry with radiation chemistry. [Laughter] He didn't know the difference. They had no radiochemistry at Notre Dame. They did have radiation chemistry. So it turns out that I wound up doing radiation chemistry in Edinburgh as my experimental work, and radiation chemistry at Notre Dame, even though my intent was to do radiochemistry.

COHEN: So you never did radiochemistry.

KUPPERMANN: I did. I took a one-month course in England in Harrow at the end of my British Council scholarship year. My advisor, with whom I did radiation chemistry, said, "Since I understand that you really wanted radiochemistry, why don't we arrange for you to take a summer course at Harrow," which is their Argonne Lab. [Tape ends]

Begin Tape 1, Side 2

COHEN: Did you go to Edinburgh first?

KUPPERMANN: I went to Edinburgh, where I stayed through—

COHEN: Did this scholarship give you travel money?

KUPPERMANN: Yeah. It paid for my travel to Britain. It paid for my expenses in Edinburgh and for my travel back to Brazil, which instead I used to travel to the United States, because I had been offered both of these—I decided to take one, get the other one postponed, and then go to Brazil.

COHEN: I see. So that was okay with all these places?

KUPPERMANN: Yes.

COHEN: You were in Edinburgh for one year?

KUPPERMANN: That's right. The British Council scholarship was also a one-year scholarship. It wasn't to go and get an advanced degree; it was just to spend some time at the university.

COHEN: How did you find that program? It must have been very different from Brazil.

KUPPERMANN: Extremely different. I found it very, very interesting. I found it fascinating. It was my first experience away from Brazil—a different climate, different sociology. I enjoyed it immensely actually.

COHEN: And Roza was with you then?

KUPPERMANN: Roza was with me. Roza didn't have a fellowship, but her parents had given us a little house, which we rented, and the rental income was enough to pay for Roza's expenses in Edinburgh. She had her degree in chemistry by then, and Nick Miller, who was a radiation

chemist at Edinburgh, was kind enough to let her work in his laboratory as a volunteer, a laboratory assistant, and she learned something. Then both of us, at the end of that stage, just before coming to the United States, spent a month at Harrow in a course that trained people in radiochemical techniques, to use isotopes—

COHEN: Finally.

KUPPERMANN: Finally. That was my first and last encounter with radiochemistry—one month. [Laughter]

COHEN: It's not very commonly known. So then you went directly from Edinburgh to the United States?

KUPPERMANN: That's right.

COHEN: You had found out by then where Notre Dame was.

KUPPERMANN: I found out that it wasn't pronounced *Notre Dam*, but that it was *Notre Dame*, and I found out where South Bend, Indiana was. My research advisor at Notre Dame with whom I got my degree, a radiation chemist by the name of Milton Burton, was kind enough to find a teaching job for Roza at a women's college across the road from Notre Dame called Saint Mary's. Saint Mary's was for women, and Notre Dame was for men. They did not interact and so on. Notre Dame was purely a men's school then, so Roza couldn't even register as a graduate student at Notre Dame. I was registered as a graduate student, but she couldn't because they did not allow women. So she instead taught chemistry. I had no intention of getting a PhD degree. I was registered as a graduate student because that was the financial aid bureaucracy. They offered me what turned out to be a graduate student scholarship at Notre Dame.

COHEN: So you were there more than one year.

KUPPERMANN: I was there initially for a year, but then Milton Burton said, "Look, Aron, I know that you don't need a PhD in Brazil, that that is not commonly done there, but the world is

changing, and you should use this opportunity and get this advanced degree. I think you'll find out that in the long run it will be important for you." I agreed. I talked with Roza, and Roza was anxious to get back to Brazil, but she agreed. So I decided to finish up a PhD degree at Notre Dame. It turns out that, towards the end of my second year, before the beginning of the third year, Milton Burton had a sabbatical coming and was going to spend a year in Germany. I would spend the year working on my own until he came back, and then continue my degree. One day, about two weeks before he left, he called me in and said, "Aron, I think you're close enough to a degree. Just finish the experiment you're doing this week and write up your thesis." That was a mad rush. I did it. I finished up my experiments, I wrote up my thesis, and handed it to him a week before he was due to leave. He read it and approved it, and I took my PhD final two days before he left. As a result, I got my degree in one year and eleven months. [Laughter]

COHEN: That's pretty good. [Laughter] The degree you didn't even think that you were working for. You must have realized also that you wanted to do research.

KUPPERMANN: That's right. Exactly. I knew that this business of earning a living in engineering and radiochemistry and so on wasn't really what would drive me for the rest of my life. I realized very keenly by then that my passion was in science. While this was going on, Burton arranged for me to be interviewed by the head of physical chemistry at the University of Illinois. I went and, after an interview, they offered me a position as an instructor as soon as I finished up at Notre Dame. All of this happened within a period of two months or so. I was not aware of it at the time, but they hadn't hired a Jew in chemistry for a decade. The head of chemistry was Roger Adams, a very, very famous organic chemist. The University of Illinois was responsible for the production of a major fraction of all PhDs in chemistry in the United States. Their graduates permeated all of the major chemical companies, of which DuPont is a keen example. But he really didn't like—he was an anti-Semite, to be very open about it—and so he simply did not hire Jews. Well, he retired that year, and his replacement had to hire—there were four or five openings because of statistical fluctuations. Accidentally, four of those five positions were filled by Jews, not because they were looking for Jews, but because the discrimination disappeared. You know some of the people. One was Martin Karplus, who is a famous chemist at Harvard. Another one was Bob Rubin. Bob Rubin is the husband of Vera Rubin, and Vera

Rubin is that astronomer whom you know. Another one was the fellow in physical inorganic chemistry, Rolfe Herber, who went on to Rutgers and is now at Hebrew University. And myself. [Laughter] Again, all of these totally fortuitous circumstances—a year before, I wouldn't have been able; a year after, there would be no openings. [Laughter] So that's how I wound up going from Notre Dame to Illinois, where I was on the faculty for eight years before coming to Caltech.

COHEN: But you went back to Brazil in between this time. I had the impression that Roza wanted to go back.

KUPPERMANN: Yeah, I did, but it wasn't in between. First of all, by then, when I finished at Notre Dame and moved to Urbana, our oldest son, Barry, had been born. So we moved to Urbana, but in order to be able to get a contract with the University of Illinois, I needed to change my visa status. I had an exchange-visitor visa, which was what graduate students had at the time, and I had to change that to a regular immigrant visa. That required one, at that time, to leave the country.

COHEN: I think it still does actually.

KUPPERMANN: Yeah, that's right. On our way from South Bend, Indiana, to Urbana, Illinois, we took a few weeks off, and drove to Buffalo, New York.

COHEN: Oh, you went to Niagara Falls.

KUPPERMANN: To Niagara Falls, to cross the border there and go to Canada and change my visa. For Brazilians there was no waiting list, no nothing. There was no problem in getting it.

COHEN: I see. They hadn't filled their quota yet.

KUPPERMANN: That's right. At the border I decided to cross by myself first and make sure everything was okay. I left Roza and Barry at the motel in Niagara Falls, and I took a bus across the border. I left the car at the motel. The Canadian immigration authority looked at my passport, and said, "Oh, are you going into Canada? But you don't seem to have a reentry visa,"

which I didn't. "Oh, yes," I said, "I don't need it." He said, "What are you going to do in Canada?" "Visit a few laboratories," I said, which I was—I was going to visit the National Research Council in Ottawa, and I had made arrangements. He said, "But how are you going to get back into the United States?" I said, "Oh, while I'm there I'm going to apply for a change in my visa." "Ah," he said, and he stamped my passport as expelled, and sent me back across the border. Officially, I hadn't crossed the border. I didn't know it, but countries that sent graduate students and other trained people with exchange-visitor visas to the United States were complaining bitterly against the brain drain that that was causing in their countries. After lots of complaints, these other neighboring countries adopted the rule that they would not allow people in for the purpose of switching visas, to cut down on the brain drain. I didn't know that. The Canadians themselves were already suffering from brain drain. Many, many Canadians in those years, in the mid-fifties, were flocking into the United States as more money was becoming available for science. So I never got into Canada, and we drove back to Notre Dame.

COHEN: Mission unaccomplished, huh?

KUPPERMANN: Mission unaccomplished. I flew to Brazil, spent a week in Brazil, got my visa changed there, flew back, and then we went to Urbana. So it was mainly the inconvenience and the expense: a return flight cost \$2,000, in 1955 dollars, which is something on the order of, I would guess, four or five times that now. It was a very large expense. So that was the only travel to Brazil. Then we went to Urbana.

Four or five years later my old assistant professor at the engineering school who told me about coolants, valence, etc.—he was by then head of the radiochemistry department of this new institute for atomic energy in São Paulo—he knew that I wanted to go back to Brazil. Well, he knew that Roza wanted to go back to Brazil. He was able to find me a position at that institute to do radiation chemistry. [Laughter] I had promised Roza that, number one, I would try to get such a job, which was a result of my inquiries, and, number two, we would only go for a year for me to try it out to see whether I would or would not be able to fulfill my objectives in life doing that. That's when we went to Brazil. By then we had three children. I was in my fifth year as an assistant professor at Urbana.

COHEN: I would like to talk more about the chemistry you did at Urbana, so maybe this is a good place to stop.

KUPPERMANN: Sure. **[Tape ends]**

ARON KUPPERMANN

SESSION 2

July 24, 2001

Begin Tape 2, Side 1

COHEN: Good afternoon, Aron. Here we are on July 24th, 2001. Welcome. We stopped talking last time about when you moved to Illinois and made the decision that your future lay in the United States and not in Brazil.

KUPPERMANN: Right.

COHEN: So tell me about Illinois and what you did there, your colleagues, and things like that.

KUPPERMANN: Well, good afternoon, Shirley. When I got to the University of Illinois, I had my choice, obviously, of what research I would like to do. I decided that the field that I had come from in terms of my graduate training, radiation chemistry, was a very complicated field. People speculated a lot about what happened when ionizing radiation and the gamma rays, X rays, beta particles, alpha particles interacted with matter and produced chemical change. The variety of things on a detailed elementary level was so broad that trying to understand the chemical effects involved an enormous amount of speculation, since each of those fundamental individual processes that probably occurred were not understood and not known. So I decided to do something more fundamental. I decided to try to study the individual elementary processes. In particular, it used to be said in those days that excited triplet states played a very important role in radiation chemistry, except that people did not have the experimental means of studying triplet states, because when you shine a light on a substance, it produces excited states of the molecules of that substance that are optically allowed. The transition from the ground electronic state to the electronically excited state has to fulfill some—

COHEN: Can I go back to something?

KUPPERMANN: Sure.

COHEN: What is a triplet state?

KUPPERMANN: Okay. Usually in molecules that are stable—that means not free radicals, but saturated molecules—the electrons appear in pairs, and in each electron pair the two spins of the electrons are opposite. In other words, electrons have this intrinsic property of spin, and in the formation of a chemical bond there are usually two electrons involved, and their spins are opposite, meaning that the total spin is zero. There is a quantity called the spin multiplicity that tries to total spin plus one, so when the total spin is zero, that spin multiplicity is one. One calls these ordinary states of matter singlets, because of that one. When you shine a light on a molecule and that the electrons absorb the light, it does not change their spin. It's the nature of the interaction process between light and matter that they have nothing that can flip a spin. So if the ground state is as usual, a singlet state, the excited state is also as usual, a singlet state. Hence you cannot detect triplet states optically, or you couldn't in those days detect these triplet states with the available light intensities. Nevertheless, these unknown triplet states were invoked as an essential aspect of how radiation produces chemical change. The idea was that, instead of light shining in—that's the main difference between light and radiation—instead of light shining in, let us say electrons shone in and produced the excitation. However, when an electron hits a molecule, the incident electron, this incoming electron, has one spin, and it can either give a kick to another electron in the molecule or it can exchange places with it. If it exchanges places with a molecular electron that has the opposite spin, the net effect is that a spin in one direction was replaced by a spin in the opposite direction, and the molecule now, instead of being in the same initial singlet state that it was in, is now in a triplet state.

COHEN: Okay. Thank you.

KUPPERMANN: It tends to be the case that when you excite molecules to triplet states, that weakens the bonding, the binding, and the molecule then tends to blow up, decompose, and produce free radicals. These free radicals, which are unfulfilled molecules, molecules with dangling bonds, are the ones that were assumed to be responsible for the chemical effects of radiation. So the triplet state intermediary was very important, and there was no means in those days of measuring these triplet states. So my first research project was to design an electron impact spectrometer which would try to measure excited states of molecules produced not by

shining light on the molecules but by directing a beam of electrons onto the molecules and then measuring the energy of the electrons after they collided with the molecules, the scattered electrons, with an electrostatic energy analyzer, a device that can detect the energy of the electrons. These electrons went in through one of these devices to make their energies be a very specific initial energy, hit the gas containing the molecules, came out of that gas, and went into a second device that measured their energy after the collision. By the difference of the two, one got the amount of energy that was deposited in the molecule, and that included the formation of these triplet states. So for the first time one had a device, a tool that permitted one to measure the presence and the energies of these excited triplet states.

COHEN: So that was one of the first things you did in Illinois, to design and build this piece of equipment.

KUPPERMANN: That's right. That was one of the three important projects I did in Illinois. The second one was, again, a matter of a fundamental process. It had been assumed up to then and postulated by a famous gas-phase kineticist, Sir Cyril Hinshelwood, who shared the Nobel Prize in chemical kinetics in 1956 with a Russian chemical kineticist by the name of [Nikolay] Semenov—they shared the Nobel Prize for discovering the first chemical chain reaction in nature that occurs when you get an explosion between hydrogen and oxygen. Hydrogen and oxygen react explosively and it's that reaction that still nowadays propels the [space] shuttle; it uses a combination of liquid hydrogen and liquid oxygen. They discovered that the explosion was due to a chain reaction—before nuclear chain reactions were discovered—this idea of a chain reaction stems from chemistry and from this work of Semenov and Hinshelwood. Hinshelwood, who was at Oxford, also proposed that when you heat up gases, like hydrocarbons such as propane, butane, and so on, they blow up into fragments. They get pyrolyzed. There were assumed to be two kinds of different steps involved in this pyrolysis. One was that scarce collisions among the molecules and the heated gas, due to the very high-energy tail of the spread of energies, could break up a small number of these molecules, producing free radicals. Then these free radicals would initiate a chain reaction of the same type for which they got the Nobel Prize, except in this case it was a hydrocarbon chain reaction. That chain reaction then made the pyrolysis very rapid. Hinshelwood felt that he was able to interrupt this chain reaction by adding

another molecule that sticks to free radicals, nitric oxide. Nevertheless, after he put a lot of nitric oxide in the heated gas, the reaction continued to occur at a much slower rate. Hinshelwood postulated or proposed that this inhibited pyrolysis was not due to free radicals anymore; it was due to a collision between molecules then blowing up into fragments that were not free radicals, but were stable molecules. This kind of process of a molecule acquiring energy by collision with others and then blowing up into two stable molecules was called a unimolecular decomposition process. Unimolecular decompositions were studied in chemistry for many years, and there was a great deal of interest. So Hinshelwood now had a whole big family of new unimolecular reactions that, he thought, were the pyrolysis reactions inhibited by nitric oxide. One of my first things in Illinois was to test that hypothesis.

COHEN: What made you think about this? Had you been thinking about these things beforehand?

KUPPERMANN: These views of Hinshelwood were normally taught in chemical kinetics courses as fundamentals of chemical kinetics in terms of unimolecular processes. They were the subjects of discussion in my research group at Notre Dame, and so I absorbed it fundamentally from that medium. I read up a little bit about it, and it gave me the impression that the foundations for the assumptions were not as well established as I would have liked, so I felt uncomfortable. What happened is that, as part of my own research as a graduate student, I was studying the effect of electric discharges on these same kinds of molecules, hydrocarbons. In order to establish the elementary mechanism of this effect of electrical discharges on chemical reactions, I did some experiments in which I discharged butane, which is a simple hydrocarbon having four carbon atoms saturated. I also discharged deuterated butane, butane having all of the hydrogen atoms replaced by deuterium. That was possible because of two fortuitous circumstances. Number one, I was being interviewed for potential jobs by the chemical industry, and in one of those—I believe it was the Standard Oil Research Laboratories—I came across somebody who had just discovered how to completely deuterate butane molecules. That was a new process, a new substance; that kind of molecule was not available previously. Secondly, in order to differentiate between these deuterated molecules and nondeuterated ones, the only method known at the time was mass spectrometry. Most people who had mass spectrometers at the time had built

homemade mass spectrometers. They had only just started to become available commercially as analytical chemical analysis tools. Notre Dame had one of the early mass spectrometers—it was actually built in Pasadena by a company called Consolidated Electrodynamics Corporation—and so I was able to produce this deuterated butane and discharge mixtures of it with ordinary butane and analyze the isotopic composition of the products of the reaction. I found, not surprisingly, that, for example, methane was one of the products. When I discharged a mixture of these two kinds of butanes, I got all possible isotopic methanes—in other words, methanes in which the four hydrogen atoms were ordinary hydrogen, others in which one of them was a deuterium and three were hydrogens, and still others in which there were two deuteriums and two hydrogens, and so on. The information that I got—how much of the mixture of isotopic methanes and ethanes and propanes—told me a great deal about how the chemical effects of the electrical discharge occurred, and that was part of my PhD thesis.

COHEN: So you had really been working on the roots of this problem.

KUPPERMANN: Right. Then it became obvious to me that an equivalent experiment should be done, not by sending an electrical discharge through these mixtures of two kinds of butanes, but by just pyrolyzing these mixtures. If, when you saturate this mixture with nitric oxide, if the residual reaction, the inhibited Hinshelwood reaction, was purely unimolecular and the butane fragmented in one single step into a methane and a propylene, there would be among the methanes totally protonated methane, CH_4 —no deuteriums coming from the C_4H_{10} butane molecules—and CD_4 coming from the equivalent unimolecular composition of the C_4D_{10} totally deuterated butanes. But there should be no mixture, isotopically speaking.

COHEN: It should go one way or the other way, shouldn't it?

KUPPERMANN: Well, in a mixture it should be both, roughly in proportion. If you start out with a 50/50 mixture of the two, then you should have roughly 50/50 mixtures of CH_4 and CD_4 , but no intermediary method. So we did it and found out that there was a scrambling of the deuterium atoms and the methane. One had CH_4 , CH_3T , CH_2D_2 , where one couldn't, one shouldn't, and that showed—that was proof positive that whatever was happening in that inhibited pyrolysis, it was not unimolecular. You obviously had free radical reactions doing the scrambling.

COHEN: Yes. Hadn't Hinshelwood already won the Nobel Prize for this?

KUPPERMANN: Yes, yes. He won the Nobel Prize. Well, he didn't get the second Nobel Prize for the unimolecular research. What he got the Nobel Prize for was the explosion of hydrogen and oxygen, and that's okay. But the unimolecular decomposition is all wrong. When I wrote Hinshelwood about these results, he said, "Yes. Those are the best experiments I have seen on that, but taking the sum total of all the results we have, I still believe that these reactions are unimolecular." He was wrong. I mean, it was just the wrong hypothesis.

COHEN: It's interesting that he answered you.

KUPPERMANN: Oh, yeah. He was a very nice guy.

COHEN: Actually, you have a good record on getting answers from people. [Laughter]

KUPPERMANN: Yeah. [Laughter] He was actually chairman of the chemistry department at Oxford. I have never met him personally, but a couple of years ago I spoke with the chairman at the time in Hinshelwood's office—the chairman's office was the same one as Hinshelwood's—and I got an interesting background on Hinshelwood's life.

So, these were two of the projects that I started with at Illinois—this testing of the unimolecular decomposition assumption, which was proven to be wrong, the building of this electron-scattering machine, and using the digital computer at the University of Illinois for, understanding radiation chemistry. It turns out that electronic digital computers were not yet available commercially.

COHEN: No. This was right at the beginning of all that.

KUPPERMANN: Right. In about 1947 or so, right after World War II, Johnny von Neumann, at the Institute for Advanced Studies at Princeton, had designed and was attempting to build an electronic digital computer which was more flexible and more totally programmable than the one that had been built during the war, called, I believe, ENIAC, for X-ray studies. He designed a very sophisticated, much better, Boolean algebra type of machine—a binary machine.

Somebody at the University of Illinois was interested in building one there also—I don't know the name of the man at Illinois; it was before my time—and he got an agreement and the plans for building a duplicate, an identical machine, in Urbana. So there were two machines being built that were identical twins, maybe starting in '46 or '47. There were difficulties with the Princeton machine—not technical ones, but getting the thing continued funding. The Institute for Advanced Studies didn't feel that that was the right place for doing such things, that they were more non-practical, basic, and so on. Anyhow, the Princeton machine fell behind, so the people in Urbana finished the design of the Illinois machine—ILLIAC [the acronym for the Illinois Automated Computer –*Ed.*]; it later became ILLIAC 1, because there were sequels—on their own. So eventually when the Princeton machine was completed, it wasn't any longer an identical twin, or a monozygotic twin—maybe it was a dizygotic twin. The Illinois machine started operating in '49, I believe. [ILLIAC 1 went online in 1952 --*Ed.*] When I arrived in Urbana in '55, it was going full blast, but it was one of the only university electronic digital computers available.

As a graduate student at Notre Dame, I was trying to understand the chemical effects of high-energy radiation on water and aqueous solutions. That was a very important topic in those days. There was a model proposed by a theoretical chemist at Notre Dame, John Magee, whom I mentioned in the last session when Pauling sent my papers to Notre Dame. He had a model in which, when you deposit energy in water by electrons and by alpha particles, slightly different things happen. By electrons you have little blurbs of free radicals formed by electrons exciting triplet states of water that decompose and form hydrogen atoms and hydroxyl radicals in a very confined region of space, in a little spur whose diameter was on the order of a magnitude of something like twenty angstroms. The H atoms and hydroxyl radicals inside such a spur had the option of either reacting with one another—some of them were just free-form water—others would form H₂, the H atom plus an H; and others would form hydrogen peroxide, an OH radical would react with an OH radical, and you would have these two so-called molecular products, H₂ and H₂O₂—or they could diffuse away from each other and react instead with something that had been pre-dissolved in the water, like a ferrous ion. These ferrous ions can prevent the oxidization by these free radicals and become ferric ions, so that you had the production of either the molecular products inside the spur or the reaction with the solvent products. This theory was based upon quantitative measurements for electrons and for alpha particles. The difference

between the electrons, where you had these little spherical spurs, and the alpha particles, was that in the alpha particles, they deposit energy so densely and intensely that the little spurs were formed in the immediate vicinity of one another and overlapped and formed a cylindrical track. So that was Magee's assumption. He said, "Well, in a spherical spur there is a better chance for the free radicals to avoid spur reactions and diffuse out into the bulk of the water than in a cylindrical track, because in the spherical spur there are three directions in which they can move away from one another, and in a cylindrical track, only two, because of the direction along the track. That would explain why in alpha particle radiation chemistry you had a larger proportion of molecular products, because they couldn't escape each other, than in gamma rays or electron radiolysis, where they had a better chance to escape." So he developed this theory, but the basic equations couldn't be solved analytically. It was not possible. He reasoned by some approximations that this would fit quantitatively. So I got to Urbana. I don't like qualitative estimates; I like to test things more accurately and precisely. As soon as I got to Urbana, I decided that the Illinois machine would permit one to solve these equations.

COHEN: Oh. So you really saw right away the potential of these machines.

KUPPERMANN: Right. I learned how to use them, started programming, and, to make the work more efficient, I established a cooperation with the wife of a colleague in Urbana. She was a mathematician and could not have a position in Urbana because of very strict anti-nepotism rules, but I was able to establish this collaboration in which she finished up the programming of these equations according to the methodologies that I developed, which I really developed as a result of a series of beautiful papers from John Todd here at Caltech. This was 1956. These papers were just a small number of years old, and in them he developed the methodology and the properties of numerical solutions of partial differential equations. So I took his ideas and developed the appropriate methods based on them, and Geneva Belford programmed them. This was one of the first applications that I did in theoretical chemistry using essentially the highest powered digital computer at the time.

COHEN: It must have been fun.

KUPPERMANN: Yeah, it was.

COHEN: But you had to punch cards? I mean, it was not so simple.

KUPPERMANN: Oh, yes, that's right. I actually did some early programming myself, and it was slow going. This early machine was very dumb. There was no software. You programmed almost in bit language. It was machine language, but it was hexadecimal characters, so each character, like the letter "a," would be a hexadecimal character in the machine and on paper tape—it was before cards; it was a paper-tape machine. It was a series of four holes, each hole being a bit, with four bits allowing you to represent a number between zero and fifteen—that's why it's called a hexadecimal character. The machine was operated on a string of hexadecimal characters, but each of these on the paper tape was just a series of four holes. One programmed in these hexadecimal characters, but when you punched them up on the paper tape you could read the individual bits you programmed up, so it was really programming at a bit level—absolutely zero software. The machine was so dumb that when you read in a paper tape to this ILLIAC 1, the first instruction was to read the next instruction. If you didn't put in that so-called bootstrap instruction, nothing happened. The paper tape wouldn't read. The machine didn't know that more was coming. It was on that level. It was a very slow and painful process, and I became addicted. I was spending all my time doing this and nothing else. I decided that I could choose between being a scientist or a programmer. I wasn't able to do both, and so that's when I dropped it. It took effort on my part, because I really enjoyed it, but I dropped it, and that's when I then associated with Geneva Belford to do these things.

COHEN: Was there much competition for time on this machine?

KUPPERMANN: No. Most people were still unaware of its potential. The number of users was sufficiently limited that you could almost request time in a one-paragraph letter and be given that time.

So there were these three projects, and finally—as I'm talking I remember—there was a fourth project. That was on quantum chemistry, as opposed to theoretical radiation chemistry, calculating the electronic properties of molecules. That was in conjunction with Martin Karplus. Martin Karplus was one of the four people who came. We shared an office in the basement of Noyes Laboratory. The laboratory in Urbana was also called Noyes, named after William Albert Noyes rather than Albert Amos Noyes. They were related, but not the same person. I had

learned quantum mechanics, but not quantum chemistry, which is the application of quantum mechanics to the calculation of the electronic properties of molecules. Martin Karplus had gotten his degree at Caltech with Linus Pauling doing calculations on the binding properties of hydrogen fluoride dimers, and so he was an expert on those. However, he had never used an electronic programmable digital computer, and both of us were interested in that. In addition, I was interested in expanding my knowledge of the applications of quantum mechanics to chemical problems. I read a series of papers guided by Martin. He acted as my quantum chemistry mentor. We decided to implement a simple project that he was interested in and that would help my learning process—the calculation of the quadrupole moment of acetylene, or whatever. So that was another project. It wasn't really my own project. I was acting on that project as a postdoc for Martin Karplus in order to learn. So those were my four projects.

COHEN: Did you have graduate students working on all these things?

KUPPERMANN: Not in the first year. In the second year, the first graduate student joined my group. Lionel Raff was his name. He decided to get involved in the designing and building of this electron-scattering apparatus. That was what I was pushing, and he was willing, and he was the first graduate student who joined my group. The second one came the following year. His name was John Larson, and he took on the project of testing Hinshelwood's unimolecular decomposition hypothesis. It turns out that it was easier to do that, because the experimental techniques had been already developed, and he finished first. So my second graduate student to join the group was the first graduate student to finish. Lionel Raff finished second. He designed and built this rather primitive machine, because in those days chemists had vacuum apparatuses that had vacuum systems, all of which were built with glass, and glass is a rather rudimentary material for constructing sophisticated apparatuses.

COHEN: Well, the first thing you did as a chemist was learn to work with glass.

KUPPERMANN: Absolutely. I spent uncountable hours as a graduate student learning how to blow glass, and my experimental work was with these glass vacuum racks. The first chemical physics type of apparatus was also a glass apparatus.

We just had a birthday party in Pasadena celebrating my seventy-fifth anniversary, and John Larson was there. To my shock, I found out that he had been retired for five years from either Ford or General Motors Research Laboratory, I don't remember which. [Laughter] He had been chairman of their physics department, had a distinguished career, and an early retirement. After he finished up with me, Lionel Raff became a postdoc of Martin Karplus', at Columbia then.

COHEN: So Martin Karplus didn't stay there all that time.

KUPPERMANN: No. Martin Karplus stayed in Urbana for four years and then moved to Columbia. I stayed in Urbana for eight years—actually seven, because one of those eight years was my leave of absence in Brazil. After Raff finished up with me, he found that the experimental enterprises were so complicated that he decided to try theory instead, and that's when he joined Karplus' group and became a theoretician. I don't think he's retired yet—he's a professor of physical chemistry at Oklahoma State [University] in Stillwater, and he has spent his research career doing classical trajectory calculations that were developed in Urbana.

COHEN: It must have been quite a powerhouse when you were there. These people you are talking about were really high achievers.

KUPPERMANN: That's right. It was really a very exciting period of time. This is a sideline, but from the point of view of a record, I think it's a very interesting one. I'll tell you how the whole field of classical trajectories, which still dominates the design of pharmaceuticals—the molecular dynamics in drug design is based partly on solving equations of motions of atoms in a complicated biopolymer. Those equations, or that approach, were developed at the time in Urbana. The initial work was done by Martin Karplus and me, but catalyzed—and this is a beautiful piece of history—I don't know whether you want me to go into this.

COHEN: Yes. Sure.

KUPPERMANN: It starts out with Henry Eyring at Princeton, and Joe Hirschfelder. He was the developer of the absolute reaction rate theory of chemical reactions—transition state theory he

also called it. He had an enormous impact on chemistry. He never got a Nobel Prize, and in hindsight this is considered to be one of the failures of the Nobel committee. There were political reasons and so on. That's not part of this story; it's an aside. Joe Hirschfelder, who became a very distinguished theoretical chemist at Wisconsin, was his graduate student. Henry Eyring had developed the early ideas of activated rate theory based on the reaction of a hydrogen atom in a hydrogen molecule. He did one of the first calculations—again, approximate ones, as they were apt to be in those years—of the forces at play between these three atoms when they interact with each other. So he had the idea of taking those forces at play and feeding them into a Newtonian mechanics calculation, assuming that the nuclei of the atoms obey the laws of classical mechanics—which they don't, but it's the best we can do. He had treated the electrons themselves quantum mechanically—approximately, but with the proper laws of nature. So he said, "Let's solve those equations of motion," just like people at JPL nowadays solve similar equations of motion to plot the trajectory of a probe to the moon. The exact same equations, except that in those days—again, you cannot solve those equations with pencil and paper. He had one of the first electromechanical calculators that were developed by the Marchant [Calculating Machine] Company at Princeton. He put Joe Hirschfelder to work on that problem—to solve, little step by little step, the equations of motion, cranking away at this electromechanical Marchant machine. You fed in two numbers of ten digits, and you flipped a switch and the machine started—clickety, clickety, clickety, clickety, clickety, clickety—until after a minute or two it finished one multiplication of two ten-digit numbers. Then you registered them and put in a third factor, a third operation, and operation by operation, painfully you did the calculation and advanced the trajectory. Joe Hirschfelder did this for three months—I checked this history, both with him and with Henry Eyring. After three months he got into what is called the transition state region of the chemical reactions, and that encouraged him. That transition state region involved a barrier like a mountain, and he got over the edge of the mountain into the center of the mountain, which actually was a volcano. It had a deep crater in the middle, and that crater nowadays goes affectionately under the name of Lake Eyring. It turned out that Lake Eyring doesn't exist. It was a consequence of the approximate methods used to calculate these forces between atoms. That's the best that could be done. That lake and that crater was important, because it's what led Eyring to develop transition state theory. If you have a region where you can get trapped inside that thing, then you can treat the reagents that are

stuck together inside that lake as if they were almost a molecule in most degrees of freedom. So it had an enormous importance, even though it was an artifact of the calculation. It doesn't exist. In some reactions it does, but in most it doesn't. So Joe Hirschfelder got into Lake Eyring, the crater, and he got trapped inside there for about two months.

COHEN: That's very funny. [Laughter]

KUPPERMANN: He went to Eyring and said, "Professor Eyring, I enjoy very much working with you. You're a brilliant chemist, and I would like to learn more from you, but unless you change my research project, I will be forced to change my research director." [Laughter] He'd had it. So Eyring put him on another problem. That calculation was published as a paper in the *Journal of Chemical Physics* and it appeared in a famous book on quantum theory, of which Eyring was one of three authors, so it's permanently engraved. That was the end of classical trajectories in chemistry for about fifteen years.

Fifteen years later, there was another graduate student at Princeton by the name of Jerry [Lejaren] Hiller, who also studied musical composition at Princeton and got a PhD in both fields. He came to Urbana in about the same year that I did as a postdoctoral fellow for Fred Wall. Fred Wall was the head of the physical chemistry department in Urbana. He later became—

COHEN: He was at UCSB. He was there when we were there.

KUPPERMANN: He later became dean of the graduate school at Urbana. From there he went to the University of California at Santa Barbara, and then to the— **[Tape ends]**

Begin Tape 2, Side 2

COHEN: So anyway, this was going on.

KUPPERMANN: So Jerry Hiller got his PhD in musical composition at Princeton and also in chemical kinetics with Henry Eyring. He came to Urbana as a postdoc for Fred Wall. He saw ILLIAC and he said, "You know, with ILLIAC we can resume the interrupted trajectory of Joe Hirschfelder of twenty years ago and see what happens." So indeed they started working on it,

and there was this first paper by Hiller, Mazur—Jacob Mazur was another postdoc—and Fred Wall, which was the first modern electronic digital computer application of classical trajectories. Fred Wall only pursued it for a little bit and stopped, but I became aware of it, and I became excited because I was interested in kinetics and dynamics. Martin Karplus wasn't interested in it at the time—he was interested in electron spin resonance and electronic properties of molecules—but I got him interested in it, and we decided to jointly do a much more thorough job than Wall was interested in. He was a statistical mechanistic, and it was mainly Jerry Hiller's interest that drove him into it, and then Jerry Hiller stopped and so he stopped. By the way, Jerry Hiller went on to use ILLIAC 1 to compose symphonies.

COHEN: Oh. For goodness' sake!

KUPPERMANN: To the best of my knowledge, he wrote the first software for composers ever produced. He knew that in a symphony, ten percent is creativity—the theme and so on—but the rest, the ninety percent of the notes, are just fulfilling very rigid rules of counterpoint dynamics and so on. He programmed up those rules and put in the theme himself, and put the rules into ILLIAC 1 one at a time—for counterpoint first, and then dynamics, and so on. He was able to convince the University of Illinois symphony to play that sequence of compositions, and they played what was called the ILLIAC Suite. I still have a tape of the ILLIAC Suite. I believe that's the first ever computer-generated—but it was really created by Hiller—it was composed by Hiller plus ILLIAC 1. He went on to become a professor of music at the [State] University of [New York at] Buffalo and died recently.

COHEN: He pursued his music rather than his chemistry.

KUPPERMANN: Right, but his chemistry generated this interest from Martin Karplus and me, and we started a joint project on three-dimensional classical trajectories on the $H + H_2$ reaction. Then Martin moved, shortly thereafter, to Columbia. We tried to collaborate at a distance, but in those days, where computer printouts were those reams of things and so on, we decided that he'd better take it over. He did, and he extended that into larger and larger molecules as computers became bigger and bigger, and that was the beginning of these modern molecular dynamics codes. The one he generated is called CHARMM. The "C" is for chemistry, the "HAR" is for

Harvard, and the “MM” is for molecular mechanics. It was the first, and is still the dominant code, and it is used by the pharmaceutical industry in designing drugs. So that all came from Eyring via Hirschfelder via Jerry Hiller via ILLIAC 1 and Martin Karplus.

At that time, when we parted ways, I decided that I didn't like using classical mechanics. It may have been the best that could be done at the time, but molecules don't care about what is convenient for humans. It marches to its own drummer, and I thought I had better learn to march with that drummer. That's when I got interested—I was already here at Caltech, so I'm skipping—in using quantum mechanics for solving these problems; and that has been and continues to be a large part of my research at Caltech. But I'll drop that for a moment to close up the Illinois business.

So in any event, those four projects—three of my own and one in cooperation with Karplus as my mentor—were what I did in Urbana. The electron-scattering machine there eventually worked. It took about five years to get that going, and indeed we started to see, for the first time, triplet states of molecules. Larson's work showed that the unimolecular assumption was wrong and, added to the theoretical project with Geneva Belford, became the theoretical foundation of the radiation chemistry of aqueous solutions. I published a lot of work there. Finally, the quantum chemistry with Martin Karplus was just a small sideline. I learned quantum chemistry. He went on to other things. I went on to other things.

COHEN: So tell me, why were you thinking about leaving Illinois? Was it because of the climate that everybody was going somewhere else? I mean, what made you suddenly decide that you were receptive to offers from other places? I know it was a time—in the sixties there was a lot of motion.

KUPPERMANN: Movement. That's right. Well, I honestly didn't decide. First of all, I did decide to go to Brazil for the year and try it out and, as I described last time, it didn't work, and with great pain and sacrifice on Roza's part, we returned. The building of the electron-scattering machine in the machine shop of the chemistry department was very painful. It was mainly glass, as I said, and mainly glassblowing. By then I had learned a little bit about metal apparatus vacuum techniques, and the chemistry departments really didn't have that; physics departments did. Martin Karplus had recently moved to Columbia and we were still in the middle of

collaborating on this theoretical work that we later interrupted. In addition, there was a group at Indiana University that was interested in helping develop a new university in Brazil. This is the University of Brasilia, and that will tie in later on with the World Bank work. This new university was going to be in the American mold, as opposed to the European mold of the University of São Paulo in Rio. Knowing of my Brazilian background, they invited me to join them in this project, and in the process they became interested in having me join Indiana University and move from Urbana. I didn't say I was available; it was just a natural thing. They made me a nice offer. I looked into it and decided that it was a sideways move; it would not improve anything—just a geographic move. It only would facilitate interactions with the University of Brasilia, because we'd all be together in one department in the United States.

By about that time, however, Martin Karplus knew I had looked into that—I think I'm doing this in the right order—and he instigated Columbia to make me an offer. I may be inverting the order of things. Martin Karplus did instigate Columbia to look into me. We were interested in continuing that project, which was quite independent of Indiana. I went there and considered their offer and decided to turn it down, mainly because it didn't appeal to me to bring up a young family in New York City. The people at Columbia then who had young children lived out in the suburbs. Westchester County was too expensive for a young professor, so the closest that some faculty there lived was in Teaneck and Leona, which was a long commute. In terms of bringing up a young family the whole environment there was not very attractive as compared to Urbana. Scientifically, the department was a little better, and of course I would have been able to continue in these classical trajectories with Martin Karplus, but when I weighed it carefully I decided not to. So these were two offers that came that I didn't look for and I just turned down.

At about that time, I organized a symposium on unimolecular reactions at the American Physical Society. At that meeting, or maybe at another one, I spoke about my work in electron scattering, so other people became aware of that. It so happened that Wilse Robinson from Caltech heard one of those talks, and Hardin McConnell, who at that time was at Caltech, even though he was considering moving to Stanford, also heard it. Caltech was looking for a physical chemist, partly because McConnell was about to move, so they recommended that they look at me. They invited me to come and give some talks, which I did on at least several topics, and made me an offer. So it is true that I was passive. It isn't that I had become restless, but it isn't

that I would be unreceptive to an offer—just that the right offer hadn't come. I was perfectly happy in Urbana. The main source of discontent was that I wanted to use the shops of the physics department, and they didn't want to have that precedent, or whatever. So that was my only source of discontent. I was very happy with having ILLIAC there. Other departments didn't have a computer like that—Columbia did, through an agreement with the IBM Watson Laboratory in New York, and so a move to Columbia wouldn't leave me behind. Anyhow, when that offer came, I looked into it. The machine shop in the chemistry department at Caltech was excellent—that was great—and of course, Caltech was very, very attractive for stature in the field and so on.

COHEN: The weather too must have been more of what you were used to.

KUPPERMANN: Yes. I had developed very strong allergies in Urbana. Our house's backyard faced a cornfield, and as a matter of fact I was becoming bedridden, the allergy was so strong. However, there was no really repulsive interaction between Urbana and me. It was the attractive interaction between Caltech and me that really catalyzed the move. So I came in '63. Maybe that's a good stopping point?

COHEN: So that's the Urbana story. I gather, as far as family life in Urbana went, that it was very pleasant.

KUPPERMANN: It was very pleasant. The kids walked to school. It was three blocks away from where we lived. The quality of the elementary school was good. The quality of life was excellent. It was a beautiful, wonderful place to bring up children. I knew that eventually I would move, because in the long range I knew that grown up children and grandchildren would not be particularly interested in staying in Urbana. So I had a larger metropolitan area in the back of my mind—but not in the heart of a city. My growing up in São Paulo, which is such a large and unwieldy city, inoculated me against wanting to live in a big city, but in the vicinity—but that was so many years into the future that that was not a driving consideration at that time.

COHEN: Was [Dr. Thomas E.] Everhart at the University of Illinois when you were there?

KUPPERMANN: This was way before Everhart. The president of the University of Illinois—of course it had only this one campus—at the time that I left, it was Jack Peltason, I believe. Maybe it was his predecessor.

COHEN: And then he came out to the University of California.

KUPPERMANN: Yes. Then he came out to Irvine. So Peltason—I'm not sure. No. His predecessor, whose name I can't remember, was the president. So Everhart—I don't know whether he came immediately after Peltason or if there was somebody in between.

COHEN: He came from the engineering school. Didn't he come from [inaudible]?

KUPPERMANN: At Cornell he was in engineering. I don't really know. But anyhow, he was not in Urbana at the time.

COHEN: I see. So the big attraction at Urbana was ILLIAC.

KUPPERMANN: That's right. Well, the big attraction was that it was the first offer of an academic job I got. Again, I didn't seek it. I was really planning to go back to Brazil after I got my PhD, and my advisor, Milton—

COHEN: Did you do any leaves then, except for the year in Brazil?

KUPPERMANN: No.

COHEN: So your leave to Weizmann [Institute of Science] was later.

KUPPERMANN: That's right. When I finished up my degree and went to Urbana, I had not yet been back to Brazil. I had not yet fulfilled my promise to Roza to try it, and that was going to take place then, except that Milton Burton said, "Look. There's an opening in Urbana. They're looking for four people. I believe you'll get it, and it would be good for your career to spend at least a small number of years there, even if you plan to go back to Brazil." So I took it on.

COHEN: So in '63 you moved out here.

KUPPERMANN: Yes.

COHEN: We'll pick that up next time. **[Tape ends]**

ARON KUPPERMANN

SESSION 3

September 13, 2001

Begin Tape 3, Side 1

COHEN: Good afternoon, Professor Kuppermann.

KUPPERMANN: Good afternoon.

COHEN: It's September 13th, 2001. So, let's go: you had just arrived at Caltech.

KUPPERMANN: Yes.

COHEN: What time of year did you get here?

KUPPERMANN: It was late August 1963. I drove across the country with my wife and three children in a station wagon. We had already temporarily rented a house until we could buy one. I started working immediately, organizing the laboratories. They had to be remodeled, and remodeling had started and was continuing.

COHEN: Were you in the old Gates building then?

KUPPERMANN: Yes. The laboratories were in the basement of Gates because a very heavy and complicated molecular-beam machine had to be constructed and assembled there. There was an enormous heat dissipation coming from an oven needed to bake the machine to get the high vacuum, so something like twenty percent of the room was occupied by a monstrous air-conditioning system.

COHEN: Did you put this together when you came, or was it already here?

KUPPERMANN: No. The apparatus itself—the design of the apparatus was started in Urbana, Illinois. The main vacuum chamber had already been ordered from a special machine shop type of company in Urbana, but it had never been shipped to Urbana, so eventually it was shipped directly to Caltech.

COHEN: So this was something you bought with your own grant money and just brought with you.

KUPPERMANN: That's right. But the remodeling costs were very significant. My recollection of the figure is something on the order of \$56,000 in 1963 dollars, which is a significant amount of money. I was temporarily put into my office—"temporarily" meaning just a small number of years, just two years. I was put into one of the Gates offices that was occupied originally by [Arthur Amos] Noyes himself. His old stand-up pendulum clock was still there. It was a large office with a large desk. The reason I mention that it was temporary is that by that time monies had already been assigned or put together for the construction of the new Noyes Laboratory. That was money donated by a man who had invented the Xerox process. His name escapes me right now. It's not Carl Anderson. [The name is Chester Carlson.—ed.] There's a plaque in Noyes Laboratory. He wanted to remain anonymous while alive, so his name was kept secret, and he didn't want his name on the building.

COHEN: He must have been a rare person. [Laughter]

KUPPERMANN: I don't remember whether it was on one of my visits to Caltech prior to moving or soon after moving that he came and visited and spoke with a group of chemical physicists who were going to occupy the building that would be called the Arthur Amos Noyes Laboratory for Chemical Physics, and still is. He was a very shy, nice gentleman. He had very interesting questions about the nature of the research. Plans were going full speed ahead, and I as well as my colleagues who would live in that building participated in designing our own laboratories. [James] Holmes Sturdivant, who was also a professor, a physical chemist from the Pauling days, had overall supervision and worked closely with the architects. So the building was put together and constructed and we moved into it sometime during '66, about three years later.

COHEN: It's a good building, isn't it?

KUPPERMANN: It's a very good building. The nature of the occupancy changed over the years. In the years between when it was opened to use and now there has been a very significant expansion of the inorganic chemistry program at Caltech which, when I came, was very, very small. As a result, right now, although I have not made an accurate estimate, I would say that inorganic chemists occupy at least half of the building, if not a little more, and the rest is chemical physicists.

COHEN: Was that a reaction perhaps to Pauling finally leaving and letting some of this other stuff come in?

KUPPERMANN: It might have been, because the inorganic chemist from Pauling's days was somebody, again, whose name escapes me. He was no longer here when I came. He and Pauling didn't get along very well.

COHEN: Verner Schomaker?

KUPPERMANN: No, no. Verner Schomaker was a physical chemist. He got along. He was one of Pauling's collaborators. This was Yost, Don Yost. I am told that they didn't get along very well, were at odds with each other. I don't know whether or not the inorganic chemistry program at Caltech was dormant as a result of that, and evolved very significantly afterwards, starting at about the time when the Noyes Laboratory of Chemical Physics opened. That's when Harry Gray came, and then slowly, over the years, more and more inorganic chemists joined the faculty, and now it's a very strong program. In those years there was Wilse Robinson, who was a chemical physicist who died just recently. Sunney Chan joined just about the same time I did. Hardin McConnell was getting ready to leave for Stanford and, unofficially, the opening that he created is the opening that I filled. Dick [Richard] Badger was still around—I don't remember whether he had retired or not, but he still came in—and there was a young theoretical chemical physicist, Russell Pitzer, Kenneth Pitzer's son. He moved to Ohio State a few years after, and he's still there. Then, within a short amount of time, two other theoretical chemists joined: Bill [William Andrew] Goddard, who is still here, of course, and Vince [Basil Vincent] McKoy, who

is also still here. Rudy [Rudolph] Marcus joined us in theoretical chemistry significantly later, in 1975. Anyhow, it was—

COHEN: A strong group.

KUPPERMANN: It was a strong group, and it was exciting to be here and make plans. The most exciting thing was the quality of the undergraduate and graduate students. I brought with me from Urbana a group of about four or five students, some were first-year students and then became Caltech students and got Caltech degrees, and others were more advanced in their research. They came with me and finished up their theses here. But they officially still got their—

COHEN: Now, how does a place feel when someone like you leaves—not only leaves, but also takes good students with them? Are there hard feelings with something like that?

KUPPERMANN: A little bit, yeah. It's unavoidable. I was given the offer from Caltech around February or March of 1963, the idea being that I would come here in August or September of '64, a year and a half after. Once I decided to accept the offer, I told the chairman of physical chemistry in Urbana my intentions, and he was very upset and he felt that it would be bad for the morale in Urbana if I lingered for a year and a half.

COHEN: He wanted it clear-cut, huh? [Laughter]

KUPPERMANN: So he encouraged me to go right away. [Laughter] So indeed I came in August of that same year, so I came within a half year rather than within a year and a half. That's a measure of the partial resentment. It was aggravated by the fact that the previous year another Urbana physical chemist in X-ray crystallography by the name of Dick [Richard] Dickerson was attracted to Caltech from Urbana, so I was the second one.

COHEN: Ah, so he felt he was getting wronged.

KUPPERMANN: That's right. They were being raided, and so they felt badly. But it is the nature of the academic world that overall tends to improve things. We have recently lost several people in chemistry to Harvard, MIT and [unclear]. It's the nature of things.

COHEN: That's how it goes.

KUPPERMANN: Yeah. That causes overall improvement in the long range, as the pressures for adding to the support and facilities comes about. Anyhow, I was very happy with two things here at Caltech. The average quality of both the graduate and undergraduate students was noticeably higher. The top of the pile, the best undergraduates and graduates in Urbana were as good as the best ones here, but the average ones were not. So it was very helpful that the average quality of the new graduate students who joined my group did improve. Secondly, one of the very, very attractive features, was that the chemistry division at Caltech had a superb machine shop built up over the years during the Pauling era, because they had a large, important emphasis on modern physical chemistry research equipment, X-ray crystallography mainly, but also electron-diffraction machines. Those were not really available commercially; you either built them yourself or you couldn't do that research. Pauling had raised the funds and developed the resources for a really first-class machine shop, which normally you would never find in a chemistry department anyplace, not even in Urbana. It was traditional that physics departments had them, because they had depended on such equipment for a long time, but chemistry departments usually depended on glass-blown equipment—vacuum lines and so on—and those don't require a machine shop; they require a good glass shop. In addition, physical chemists had to learn how to blow glass, because those vacuum racks were built directly in the laboratory and frequently broke and developed leaks. So unless a graduate student knew how to blow glass, he really was not effective.

COHEN: So are there professionals who run this lab? It's not the professors? They just go in and order the equipment and somebody in the machine shop builds it?

KUPPERMANN: Yeah, that's right. Well, the way it used to be—and I'll mention this now—is that you sat down and, depending on the complexity of the equipment, you made a sketch and explained it to somebody at the machine shop who was a mechanical engineer. He'd transform

your sketches into machine-shop drawings and then the instrument maker—the machinist—would build it. The professor and his graduate students kept in very frequent contact, daily at times, to make sure that what was being built was really what was intended and so on. Over the years, this type of operation became more and more expensive. The general funds needed by the division to support it did not grow with the demand, so more and more of this type of work had to be paid for with research grants. As the hourly wages and so on increased, it eventually became impractical. People then started getting bids from outside machine shops that had larger volumes of work and could do this more effectively because they would live by tighter time schedules and so on. So our shops no longer build the type of complex physical chemistry equipment that they used to, and as a result the shop is much less significant. It's mainly used for small pieces of equipment, rather than big ones, and maintenance. However, in those years they were building the big pieces of equipment, and that was enormously important for my own work.

COHEN: So you arrived with four or five students already. You hit the ground running, so to speak.

KUPPERMANN: Yeah. The first effort was to install the equipment that I brought with me from Urbana. That equipment had been purchased with federal research grant funds—at that time it was still the Atomic Energy Commission. Universities had agreements with these federal agencies that equipment that was purchased or constructed with grant funds would move with the researcher, so there was no major difficulty in getting Urbana to agree to that. Within six months or so, the equipment that had already been functional in Urbana was up and running.

COHEN: Oh, that's very good. Did you have to start teaching at that time? You came a year early, so maybe they left you alone. [Laughter]

KUPPERMANN: I started teaching immediately. In the fall of '63 I started teaching two courses, to the best of my recollection. One was the undergraduate physical chemistry course that had been taught with a certain structure up to then. I had introduced a very different one in Urbana by beginning with quantum mechanics and statistical mechanics, and then moving to thermodynamics with a strong basis on the molecular structure of matter.

COHEN: So Caltech students can handle quantum mechanics right from the beginning?

KUPPERMANN: They didn't know quantum mechanics and physical chemistry. They had had a small smattering in physics, but this course was organized so that the first thing I did was teach them quantum mechanics at the level that would be needed for the understanding of physical chemistry. It was not a major problem because as undergraduates they had a very good background in mathematics and physics. It's just that it previously had not been done that way. Previously things were a little more classical. So I enjoyed that. I also taught a graduate course in statistical mechanics, which is not my field. I had become interested in learning more statistical mechanics while I was in Urbana, so I took some courses in the physics department there that were really very up-to-date state-of-the-art courses, and I enjoyed learning it. So I just plagiarized. I took a course that I took as a sit-in faculty student there and introduced it here.

COHEN: Ah, but that's the best way to really learn something. So your teaching was certainly less here than it was at Urbana, I would think, but maybe not.

KUPPERMANN: A little less. I believe that in Urbana I taught a year's course every year; I taught the undergraduate physical chemistry course, which was a year's course. Here in the beginning I taught about the same amount, because I wanted to get these courses going. On average here the teaching load in a year or two was just two out of the three academic terms per year, and no summer, whereas there it was a full academic year, and no summer unless you wanted to earn some more money during the summer, and perhaps a little more. So my average teaching load did indeed decrease, but I have always enjoyed teaching, so that was not something that was an important, attractive feature for me.

COHEN: Well, I think you're rather unique. You still enjoy teaching.

KUPPERMANN: Yes, I still am teaching.

COHEN: If not, you would have retired. [Laughter]

KUPPERMANN: That's right, and I've been teaching at least two terms a year for time immemorial.

COHEN: A long time. Did your family adapt to Pasadena right away?

KUPPERMANN: Yes, my family enjoyed Pasadena. It was a major difference climate-wise. The thing that we noticed most was that the children started consuming a larger number of shoes and tennis shoes per year.

COHEN: Ah. They were more active here.

KUPPERMANN: In Urbana in the winter you'd spend most of your time indoors. Outdoors, you'd go out with galoshes.

COHEN: Now, is this weather more what you're used to in Brazil? Do you have a winter in São Paulo?

KUPPERMANN: There's a mild winter. It is similar to São Paulo, with one very significant difference. São Paulo is a very humid climate, whereas Pasadena is on the average much drier. I was very sensitive to humidity, and I still am, so for me the climate in Pasadena is much more pleasant than in São Paulo.

COHEN: Oh, very good. At least you didn't miss the winter. Well, none of us missed the winter when we came. So you very quickly got into life here. I see that after half a dozen years, or seven years, you took your first sabbatical leave.

KUPPERMANN: That's right. My first sabbatical leave was in 1968, which was—

COHEN: Five years.

KUPPERMANN: Five years. That had been prearranged, because I hadn't taken a sabbatical from Urbana. I had taken a year's leave of absence without pay to go back to Brazil, and that was in

1960. So come '68, I was ready for a sabbatical. When we discussed the conditions and terms of my accepting the Caltech offer, that was one of the things discussed. They told me then, and it is still true now, that there is no official sabbatical policy here. Any faculty member at any time can request a year's leave of absence with half pay or a half-year with full pay as long as he or she justifies it appropriately and the division chairman and the provost approve it. That's all that is required, and they told me that.

COHEN: Many people never go away.

KUPPERMANN: Yeah, a large fraction of the Caltech faculty. So I spent the first half of my first sabbatical at the Weizmann Institute [of Science] in their isotope department. They were doing work that I was interested in. The other half was in Amsterdam at the FOM Institute for Atomic and Molecular Physics where, again, they were doing things that I was interested in here. I had built an addition to a sophisticated cross-molecular beam machine, another apparatus that was a low-energy electron-scattering spectrometer, and that was going very well, in 1967 or so. In '66 or '67 it started producing its first results. As I have already mentioned in a previous session, we were able to detect these low-lying triplet states of molecules, some of them for the first time. Over the years we discovered a few hundred new electronic states of molecules that were involved in these triplet states. They were doing something related in Amsterdam, but not the same thing.

COHEN: So you lived in Amsterdam, then, for six months.

KUPPERMANN: Yeah. I spent about four or five months in Amsterdam.

COHEN: You must have enjoyed your six months in Israel.

KUPPERMANN: Yes. The six months in Israel were—

COHEN: Had you been there before?

KUPPERMANN: Just for a short period, a short visit in 1960 for a month or so, mainly as a tourist.

COHEN: So if you were there in '68, that would have been after the Six Day War; and it was quiet then.

KUPPERMANN: That's right. We arrived in the fall of '68, so that was one year after the Six Day War. The restrictions on acquiring automobiles in Israel—the financial difficulties were great, they were very heavily taxed, and if you bought one, then to sell it was very difficult. After some investigation it turned out that the cheapest way to have a car there, which we needed, since we had four children, was to ship my car out from Los Angeles and then ship it back.

COHEN: Oh dear.

KUPPERMANN: It was incredibly inexpensive. It cost \$400 to ship it each way, which even in those years, if you normalize it to current dollars, was something on the order of \$1,200 each way. For \$2,400 I could have my own car for a year without any—

COHEN: So that's what you did.

KUPPERMANN: So that's what we did. In that car we traveled throughout the West Bank, to all of these points of conflict right now—Ramallah, Nablus, and Jenin. I drove and visited with my family of four children, and there was no hostility that one could detect externally. The Palestinians had not, for time immemorial, had a country of their own. Prior to the establishment of Israel, they lived under the Ottoman Empire jurisdiction for hundreds of years, then they were under the British Mandate for another forty years, and then this part, the West Bank, was under Jordanian jurisdiction from '47 or '48, once the British went out, to '67. So that's thirty years, and now it is under Israeli jurisdiction. It was very mild in those years. The feelings of nationalism and of wanting a country had not yet evolved to the level that it is at now. There was always some tension, but there was no major hostility. They lived their lives; the Israelis lived theirs. It was peaceful enough for me to not feel that I was endangering my family by visiting the West Bank.

COHEN: We drove around in the early seventies.

KUPPERMANN: Yeah, same thing.

COHEN: How was it scientifically? Was it a worthwhile six months?

KUPPERMANN: Yes. I interacted with a few Israeli scientists, chemical kineticists, in a positive way. They actually made me an offer. They wanted me to move to the Weizmann. After mulling it over for a while, I decided that I had already moved the family too much, and decided not to, but I kept a close interaction with them.

COHEN: The author who wrote this book, *Passion to Know* [Mitchell Wilson, *Passion to Know: The World's Scientists* (1972)], he likes the Weizmann Institute.

KUPPERMANN: Does he? To be honest, I haven't read it. [Laughter] You know more about it.

COHEN: He said it's one of the ten best establishments in the world; he doesn't say in the western world, he says the world.

KUPPERMANN: The Weizmann Institute is a very unusual place because it is a world standard for a cutting-edge institution; it was already in those days, and is even more so now. It is located in a very old community, Rehovot. Many Yemenites settled at the southern edges of Rehovot after the "magic carpet transfer" from Yemen to Israel took place in '50, '51, so there are many Yemenites who lived, and still do, in Rehovot. Due to our big family, we shipped big crates, and the crates were taken apart inside the woodshop of the Weizmann Institute. When it came time to come back to Pasadena, it was necessary to put all of our stuff back in the crates, and it was easier to take our stuff from our apartment to the woodshop of the Weizmann, where the crates still were. It turned out that the easiest way to do that transportation was to hire a horse-drawn—not quite a buggy, but a platform—a big platform with a horse pulling it. It was very, very broad, much broader than a regular automobile. We just piled all our stuff on top of it, and that horse-drawn transportation took it to the Weizmann. The Yemenite man who was doing it didn't know exactly where to go, so I showed him the way with my Dodge Dart car. Our three oldest kids rode their bicycles—because they had to be crated—one on each side and one in the back. So you had this procession. You can imagine it vividly.

COHEN: Did you take some pictures at least?

KUPPERMANN: No. [Laughter] I'm sorry, Shirley.

COHEN: That's too bad.

KUPPERMANN: It was marvelous. We barely were able to squeeze through the gate of the Weizmann, given the width of this conveyance. It was a marvelous contrast of the old and the modern. They say that the founding fathers of the Weizmann Institute had great foresight in locating the institute so conveniently close to Israel, because in those years it was not Israel. It was a modern American-style campus, with its lawns and structures and so on, whereas the surroundings were still very Middle Eastern and old fashioned. So it is not Israel; it's located close to Israel. [Laughter] Nowadays that's no longer an appropriate statement, but in those years it was.

COHEN: Well, those were quite some years ago. This was still the first generation of those Yemenite people.

KUPPERMANN: That's right.

COHEN: So then did you have to take all this stuff to Holland with you?

KUPPERMANN: Yeah. The crates were shipped by boat to Holland, and then they were shipped from Holland back to Pasadena.

COHEN: Poor Roza. [Laughter] Holland must have been quite a contrast.

KUPPERMANN: Yes, it was. Everything was very different from Israel, but the whole year was very enjoyable and very promising. Scientifically, I sat down and started working on very different problems. That's the nice thing about sabbaticals. You don't go to a sabbatical to keep on doing the research you're doing in your original institution, because the best place in the world to do that is there.

COHEN: To stay where you are.

KUPPERMANN: So I used my detachment from committee work and work, and from other activities, to sit down and think with pencil and paper. What I started doing there, which was theoretical work, was in the long run what I wound up doing, what I am still doing now.

COHEN: I guess that's the idea. As you say, that's the idea for a sabbatical leave, to refresh yourself.

KUPPERMANN: Right.

COHEN: So you came back after the year, and you started doing this different work. So what was that?

KUPPERMANN: Well, I started slowly. That was the quantum mechanical theory of chemical reactions, how to predict from the equations that govern molecules—equations of quantum mechanics, the Schrödinger equation—how to use that to predict the cross sections and rates of chemical reactions. It was understood that that should be possible because these laws of nature are the ones that should govern molecules, but the exact way to do it wasn't well understood by chemists. Nuclear physicists understood how to do that for nuclei, and developed some formalisms, but they were not quite applicable to molecules because the forces involved were different. The interaction forces—the Coulomb's laws that governed the interactions between electrons and nuclei that form molecules—were known exactly, whereas in nuclei the forces at play between the particles that make up nuclei—protons, neutrons, and nucleons—were not known. So the methods developed in nuclear physics were not really applicable to chemistry. Chemistry really required thinking from scratch. That's what I started thinking, and then doing some theory, and some of my graduate students did some calculations. It slowly evolved into something that we understand quite well conceptually. In practice it is limited by the fact that, even for small molecules, the computational effort needed to do a prediction that can be replicated in the laboratory is an enormous computational effort. So by necessity in the early years the systems were very simple and the calculations were adapted to the limited speed of computers.

COHEN: So you were coming back to your love of computers now.

KUPPERMANN: Yeah, right. Not only that, but then, roughly seven or eight years after returning from Israel, we were doing the first calculation without any approximations on the reaction, a very simple reaction on which I had done experiments—hydrogen atoms with hydrogen molecules, or hydrogen atoms with deuterium molecules. Some of those experiments are the ones alluded to, but I wanted to be able to understand them well and predict the results of such experiments. That brought about—I don't remember whether we talked about it or not—my use of the Ambassador College computers.

COHEN: I think you said that you were looking for big computers. Were they inviting people from Caltech to come use the computers?

KUPPERMANN: No.

COHEN: How did you get in there?

KUPPERMANN: Well, it was very interesting. Caltech had a big computer, but in order to use it I had to pay \$300 an hour. The institute was trying to make the computer center break even, and the computer was very expensive. It wound up to be \$300 an hour, in 1973 dollars. That would be, roughly speaking, \$1,000 an hour today. I needed hundreds of hours. It wound up that this calculation that I'm referring to, once it was done and over, consumed about 1,000 hours. That means \$1 million in current dollars, \$300,000 in 1973 dollars, and I couldn't afford that. I found out accidentally that Ambassador College had a duplicate, a computer exactly equal to Caltech's. I found that out by a very fortuitous circumstance. Ambassador College celebrated Jewish festivals. They had a Sukkoth Festival during which they closed the place up and went away on vacation as a group and had Israeli folk dancing. An Israeli folk dancer trained there, and he came to Pasadena once a week. We were preparing for the bar mitzvah of our second son, Nate, and we had used that dancer in our oldest son's bar mitzvah, so we wanted to speak with him. The most convenient place to speak with him was when he came to Pasadena for his night dancing. We spoke with him and found out from him that Ambassador College had a big computer.

COHEN: That was for their mailing list.

KUPPERMANN: That's right. They received donations from about four million donors all over the world, and to have the bookkeeping and the backgrounds of each donor—when they gave money, how much, and so on—required a huge computer. It didn't require them to use it at night or on weekends, just during the day. Once I found that out, I tried to make arrangements to see whether they would allow me to use it at night. At the time I had an Israeli postdoc, Michael Baer, who was working with me on the early stages of ab initio theory—a theory with no approximations. I knew that they had a special interest in Israel; they wound up funding the excavations on the southern wall of the temple. I invited them to come to Caltech and have lunch with me, and to show them my labs. During lunch they asked me what I thought about the biblical account of the origin of life. I knew that my access to their computer depended on an appropriate answer to that question. I said, “Well, I am not a biologist, and my work is not related to that, however I can say that in the scientific community some believe in it and some don't,” which is absolutely one hundred percent true. I have orthodox friends who take the Bible literally.

COHEN: And I've taught with some science teachers who didn't believe in evolution.

KUPPERMANN: Then the conversation moved on to something else, so apparently I passed that test. I took them to the lab to meet my group, and my students, and in particular this Israeli fellow, because I felt that that would be interesting for them. I go into the lab and I see this fellow with a tie and a coat and properly dressed, and I asked him, “Have you seen Michael Baer?” Then I said, “Oh, I'm sorry, Michael.” It was he. He had cut his long hair short, put on shoes rather than his sandals, and put on a tie and a jacket, which I had never seen on him before.

COHEN: He was wearing his Ambassador clothes.

KUPPERMANN: Yeah, he was in his Ambassador attire. We chatted, and he passed that test, and thereafter I was able to use their computer.

COHEN: So you didn't pay for it?

KUPPERMANN: No. It was very inefficient, because they didn't want me to be inside their computer room with all of these mailing lists, which were a trade secret. So the way we did it—those were the days of the IBM punch cards--so Michael, and later on George— **[Tape ends]**

Begin Tape 3, Side 2

KUPPERMANN: We would hand in the box of cards on Friday afternoon, before their computer center closed around five o'clock, and come back Monday morning to pick up a big, thick stack of printouts. If by any chance their operator fed those cards in wrong, or one card fell on the floor, the weekend was lost. It was very, very inefficient.

COHEN: Oh, so their operator fed the cards in. They didn't let you go in there.

KUPPERMANN: No. Not only that, but then he went home, and the computer center was closed for the weekend. The machine kept on going. If we were lucky, everything went well and we would get ten, fifteen hours' worth of computing. If we were unlucky, we'd get zero. So it was a slow, painful operation. The same was true for these Sukkoth vacations. We had to prepare runs that could in principle last for ten days, which involved an enormous stack of IBM cards. Again, if they were read in improperly, that was the whole ten days lost. It took us a year to run these 1,000 hours, from which the actual production was 300 hours. It was worth it, however, because we did the first principles calculations on the cross section and rates of a chemical reaction that helped us a great deal in understanding how these chemical reactions took place.

COHEN: When you wrote this up, did you give Ambassador College credit?

KUPPERMANN: Yes. Every single paper that was based on those calculations had a simple statement in the acknowledgement section saying, "and we thank Ambassador College for the generous use of their computational facilities." These were the first calculations ever done, and now they are considered classical and of an historical nature. The first paper was published in 1976, by George Schatz and myself. On the recent twenty-fifth anniversary of those calculations an English colleague, David Cleary, wrote up a special paper on the history of these calculations by my graduate student, George Schatz, and myself. The story is that from the very beginning

we were interested in understanding how chemical reactions occur at a chemical level and the first involvement of that were these experiments that we talked about. The next step was to try to do the same thing theoretically to see whether the basic laws of quantum mechanics really did explain all of chemistry. We knew by then that it explained the structure of molecules quite well, but we did not know whether it correctly explained chemical reactions quantitatively. It was believed that it did, because if it didn't, then there was something fundamentally wrong. Still, that idea or that type of powerful nature of quantum mechanics had not been tested. This was the first complete test.

COHEN: You must have been very satisfied.

KUPPERMANN: Yes, it was very satisfying. Over the years it has evolved from initially just a hydrogen atom with a hydrogen molecule—so there are three atoms—to more general three atoms, and then more recently—and this is going on now—to four atoms, and you may think, well, the interesting thing would be much bigger molecules, let us say biological molecules—proteins and DNA. If it takes you twenty-five years to go from three atoms to four atoms, what future is there in this approach? Well, it's interesting. There is a very important future. Namely, when you have three atoms, you break one chemical bond between two of the three atoms and make a new chemical bond between the reagent atom and the new atom formed when you break the old bonds. So it's what is called a three-center reaction—you break one bond and you make one bond. When you have four atoms, you break two bonds and you make two bonds. When you take two large molecules, let us say enzymes and proteins, even though the molecules are very large, the chemical reactions occurring in a significant number or fraction of those are all three- or four-center reactions. You still only break one bond and make a bond or break two bonds and make two bonds. The rest of the molecules are like spectators in a wedding. The real action is going on between the bride and the groom, and the audience gives moral support and cheers. The audience is, to a certain extent, important, because this is a social event, the wedding, but the most crucial part is the bond being made between the partners. It's the same thing with molecules. The most crucial parts are the atoms directly involved in making and breaking bonds. The effect of the rest of the molecules is much less important. It's what is called in technical terms perturbations of the main process. So in studying the reaction between

large molecules, as long as you do the part of the theory involving the three or four atoms among which bonds are being made and broken, you can inject the effect of the rest by much less rigorous techniques. Computationally that is not enormously expensive. So these ideas and these approaches are now being extended to much larger molecules, and we're starting to do work on that right now. So this is the last chapter. [Laughter]

COHEN: Is this going on just here, or are there other places that are doing this kind of work?

KUPPERMANN: There are other places that are doing it in which they try to use the rest of the molecules approximately, but the reaction itself is also being done very crudely, because that part is very expensive, and very few places know how to do that part well. This is one of the relatively few places in the world in which, especially for the four atom or four-center reactions, they are done in a detailed way. There are only four or five places in the world that know how to do that, and to the best of my knowledge, we are the only one trying to marry that with the rest.

COHEN: So you continue just as excited as ever. [Laughter]

KUPPERMANN: Yes. I enjoy the work enormously. Slowly, over the years, we have shifted from—as soon as we arrived at Caltech, I was really just doing experiments, very important fundamental experiments in electron scattering, the mono-energetic reactions of these H atoms and so on, and then evolved into doing photoelectron spectroscopy, which was an outgrowth of the electron scattering. The theoretical effort in understanding the making and breaking of chemical bonds started slowly, and it started evolving. As time went on, in the late seventies, we were doing half theory and half experiments. In the late eighties or early nineties, the switch over to doing only theory was complete, because we are still interested in the same problems that have not been solved. It turned out that the evolution of the theoretical understanding, hand-in-hand with the growth of the power of computers, made the theoretical approach more productive than the experimental one. The same questions could be answered more reliably and in much greater detail than by doing even the most sophisticated experiments—for very, very simple systems involving three and four atoms. Once you can do those, you can extend that to much more complicated systems. The problem is to understand the making and breaking of bonds in chemical reactions. The tools are whatever is appropriate to answer the questions posed, and

those tools are the ones that changed over the years. But the problem is there, and hopefully we're approaching the state in which it's being solved.

COHEN: So now let's talk about your citizenship here—I mean, your research, of course, and your teaching. More was expected. Was there any particular interest you had here over the years as far as committee work?

KUPPERMANN: Yes. I had an interest that started in Urbana, which is the responsibility of a university to the community in which it resides, and to society in general. During my last few years in Urbana, I was involved in organizing a group of faculty interested in nuclear weapons policy, the dangers of these weapons, and what could be done to avoid expanding and generalizing their use. I became interested in these societal problems. When we moved to Pasadena, the nature of those issues had changed. By then the test ban treaty had been signed and that problem was more under control, but it was becoming obvious that the health of universities that are embedded in cities was dependent on good relations between the university and the community. In Pasadena the problems in the black communities in east Pasadena and northwest Altadena were becoming more severe. Pasadena had a large black population, as opposed to its neighbors such as Arcadia and Glendale. Of course, Pasadena was from very early times very open to blacks, mainly because it was a wealthy community and the rich people needed servants, so they brought their servants. The servants didn't want to come without their families, and the wealthy magnates didn't want the family of the servant living in the same, although very large, house with them, so that's why the families lived in northwest Altadena. That was the beginning of the black community. Arcadia and Glendale never had a significant black community, and the restrictions on real estate and whatnot were sufficiently severe to hamper it. Well, when Harold Brown came to Caltech in '69, I was a member of the faculty board and I pointed out to him that Caltech needed to keep in contact with the community and be aware of the issues involved. He appointed a committee for relations with the community on which I served as chair for many years, for seven, eight years, so I was very active during those times. We brought the vice-chancellor of the University of Chicago here to help us become informed—I think Levy was his last name, but I forget. This was in the early seventies, and the University of Chicago was having much more severe problems, because they were right inside

the black community. We established links with the mayor's office. So that was an important activity, which was centered on Caltech but related to the community.

COHEN: Who served on that committee? Was it just people who were interested in this problem?

KUPPERMANN: Well, I would have to go to my files to refresh my memory on the other members of the committee. My recollection is that Norman Brooks was on it, and perhaps Jim Morgan, but it's been so long—it's been about thirty years—that I don't quite remember.

COHEN: Do you think you accomplished anything?

KUPPERMANN: After a while I thought that it would be appropriate for somebody else to take over. Ned Munger took over for me, but the focus and the concern with the issues involved shifted from the committee to the administration. The administration became larger and there were people there who keep an eye on this thing. In those years it was Jim Black. He was a member of the administration and we'd interact strongly with him. The whole societal concern shifted away from these. These were still—

COHEN: Innocent days.

KUPPERMANN: Innocent days. Yeah, that's right.

Another activity that I was involved in had that character—those were the days in which the schools in Pasadena were becoming more and more segregated. We had a federal judge in Los Angeles, Manuel Real, who was trying to do something about it. There was an issue that in some schools the majority was made up of minorities. Judge Real appointed a committee of Pasadena citizens, and I was a member of that committee.

COHEN: That was as a citizen?

KUPPERMANN: That was a mixed thing. Each person represented, unofficially, a certain constituency. I don't think I represented Caltech in any way, but the fact that I was on the

Caltech faculty was, I think, part of the reason I was appointed by Judge Real. Most of our meetings were in the Millikan Library, in the Board of Trustees room, which I arranged. So the administration was aware of these activities, but I didn't represent Caltech directly. That committee attempted to come up with recommendations for Judge Real on how to deal with the problem, which he thanked us for and adopted. In the end the idea that you should not have schools in which a majority was a minority never worked. We were trying to stop white flight.

A third activity of a non-scientific nature was the matter of computing facilities at Caltech. That was in the years of Murph [Dr. Marvin] Goldberger. It was realized that super-computers were coming into play, and Caltech had none. There were no super-computer centers yet at the National Science Foundation, or those were incipient, and we had to scrounge for computer cycles at the national laboratory. Murph appointed this committee that I chaired for two years. That was in the early years, in the early and mid-eighties, in which parallel computers were being developed at Caltech and elsewhere. They still were not available commercially. The question was what Caltech should do in terms of fulfilling the computing needs of its faculty. This committee came up with the recommendation of a dual tier—we needed a good commercial vector computer and we needed significant activity in parallel computing—and that report was approved by Goldberger. However, before it could be implemented, Goldberger, and Robbie [Rochus] Vogt, who was his provost and also a strong supporter of this, both left. In subsequent administrations we had to start convincing the new administrations from scratch of this need. Eventually they slowly became convinced of the need for the parallel computer, but not that Caltech needed a big state-of-the-art commercial Cray vector computer. The parallel computer slowly took root and evolved eventually into what is now called the Center for Advanced Computing Research, CACR, that has a significant parallel computer, but that is not really state of the art any more. At one time the computer we were able to put together was the best and fastest in the world. It was still not commercial. It was made by Intel, but it was a prototype, it was a Delta computer. So I've been involved in the computing activities on campus for a large number of years, and I am still a member of the computing advisory committee. I feel that we had an opportunity to become the country's best center for parallel computing activities, and that we didn't make full use of that opportunity.

COHEN: That's because you didn't get the encouragement from the then-administration.

KUPPERMANN: That's right.

COHEN: That's too bad, because it remains a problem.

KUPPERMANN: That's right.

COHEN: Well, it sounds like a lot of work, all of the committee work.

KUPPERMANN: It was a lot of work, but I enjoyed it, and I felt it was important for the institute. In addition, I had a vested interest for my own work.

COHEN: I think we'll stop here. **[Tape ends]**

ARON KUPPERMANN**SESSION 4****September 25, 2001****Begin Tape 4, Side 1**

COHEN: Good afternoon, Professor Kuppermann. This is September 25, 2001. Welcome. We are speaking about your many activities outside of the institute. Do you want to continue with some of these other activities of yours?

KUPPERMANN: Sure, I'd be glad to. There have been activities associated with international issues. They started rather early in the game. About five years after I was here, in 1968, Carl Djerassi of Stanford University came up with the idea of creating a cooperative program between the United States and Brazil to help improve, develop, and modernize graduate education and research in chemistry in Brazil.

COHEN: What was his connection with Brazil?

KUPPERMANN: There was none. He had a connection with Mexico, where he did research with Alejandro Zaffaroni who had a drug manufacturing industry there.

COHEN: What was the name of that?

KUPPERMANN: The name of the man is Alejandro Zaffaroni. The name of the company was Syntex. There he did basic research involving the development of the birth control pill, and that was very successful. Zaffaroni opened up another company in the United States, headquartered in Palo Alto. What happened, as one would expect, is that Carl Djerassi was one of the co-owners of this subsidiary. It was called ALZA—ALZA being the first syllables of Alejandro Zaffaroni's name. I do not know exactly what the timing of that ALZA Company was, but the point is that by then Carl Djerassi was on the faculty of Stanford and had seen the potential for Latin-American scientists and what they could contribute. He felt that the next country after Mexico should be Brazil, because of its size, its human potential, and the number of trained scientists that it had. As a member of the National Academy of Sciences, he tried to develop this

joint program. He did that, and he enlisted the help of Atlantic Richfield Oil Company. He identified five areas of chemistry that needed reinforcement in Brazil, five American scientists who would be willing to take part in a cooperative arrangement, and five counterpart Brazilians, and created this group of ten people—five Americans, five Brazilians—who would get involved with this effort, with the five Americans each sending an ex-graduate student or postdoc down to Brazil. They would stay there, presumably with their families, for a period of about three years, and get some research started in those areas. The Americans—let me see if I can identify them—in addition to Carl Djerassi there was Fred Johnson at Stanford, Harry Gray from Caltech, George Hammond here at Caltech, myself—oh, and there was another one—at Michigan, Charlie Overberger who was a polymer chemist. So the areas were photo-organic chemistry represented by Hammond, synthetic chemistry represented by Johnson, polymer chemistry by Overberger, inorganic chemistry by Harry Gray, and physical chemistry by myself. Carl himself did not get involved in the creation of the groups, but he oversaw the whole thing. Then there were Brazilian counterparts in these areas. So the planning got started in 1968, the program started in 1969, and it lasted until 1977, for eight years. Initially five groups each were developed at the two strongest universities, the University of São Paulo and the Federal University of Rio de Janeiro. Some of them took, and others didn't. About six or so of these groups took.

COHEN: That's very good.

KUPPERMANN: That's right. It was a high yield. Some of the postdoctoral fellows stayed permanently and are now professors at one of these two universities.

COHEN: You mean people from São Paulo, or from Brazil?

KUPPERMANN: No, the people from the United States.

COHEN: Oh, they stayed at their universities.

KUPPERMANN: Yeah.

COHEN: Usually it's the other way around.

KUPPERMANN: They married Brazilian women and— [Laughter] Of course some Brazilian young people also got involved and are well established now in the program. Some years ago it celebrated its twenty-fifth anniversary—that was in '94. They had a meeting of the Brazilian Chemical Society at which some of the graduates of these programs spoke, and they assessed their overall impact on chemistry in Brazil, and it has been very significant, because their graduate students who graduated under this program are now professors in other Brazilian universities. This was a period of expansion of the number of federal universities, and so there is essentially no university in Brazil that doesn't have on its faculty a professor of chemistry who got their training in that program. That was very important, because chemistry in Brazil was very old-fashioned. It was established in Brazil in the middle or late thirties by two German immigrants who were fleeing Nazi Germany. Unfortunately, they were of the old German school that was by then in decline, but that's what took root in Brazil. In the same period of time, in the mid- or late thirties, physics got started in Brazil, mainly at the University of São Paulo. That was also through immigrants. The main immigrant then was a White Russian by the name of Gleb Wataghin who came from Italy—he fled Communist Russia, became established in Italy and was one of the early cosmic-ray physicists. When he moved to Brazil, modern physics started in Brazil. So physics in Brazil has always been healthy and modern, whereas chemistry was old-fashioned.

This program, which was joint between the Academy of Sciences in the United States and the Brazilian NSF [National Science Foundation], which is called Conselho Nacional de Pesquisas—it goes under the acronym of CNPq—this partnership really led to the modernization and reinvigoration of chemistry in Brazil. Carl Djerassi was chair of the group for the first four years, and I was chair of the group for the next four years. Those were the days when Brazilian protectionist policies limited the importation of scientific equipment. Nevertheless, we needed to establish these modern research groups with modern equipment. The American members went twice a year—the senior professor—the postdocs were there all the time. Whenever we went to Brazil, we tried to smuggle in equipment. I remember one time I smuggled in—I didn't smuggle; I mean, I went through customs—it was a big, flexible hose with flanges at the end that was part of a metal vacuum system for an electron-scattering spectrometer. I carried it under my

arm, and I was expecting the Brazilian customs people to complain. They asked what it was, and I said it was part of a vacuum system, and they said, “Oh,” and let it through.

COHEN: [Laughter]

KUPPERMANN: Without doing it that way, the paperwork and the red tape was horrible. It took six months to get anything through. The organic and synthetic chemists smuggled important chemicals in their briefcases. So it really was an organized smuggling operation in which nobody was ever turned back or caught. That helped to get these research efforts going, because if you had to order a chemical for chemical synthesis, and had to wait six months for it to arrive, then that would kill the project. So it was very, very useful, very influential. It came to a natural end after eight years, as it took root.

In the early eighties the World Bank started getting interested in science and technology as a developmental tool, as a tool that would accelerate the economic development of countries. They decided that modern economy was heavily dependent on technological improvement and that you couldn't transplant technology into a country unless there was a human resource base capable of absorbing it and adapting or utilizing it, and that required well-trained people. Well-trained people meant people trained at a graduate level in research, because these are new techniques, new science was involved. Brazil did not have a pool of modern technological people. The World Bank had been doing that very successfully for a year or two with South Korea—the training or support by the World Bank of activities and research in science and technology in South Korea. That was the World Bank end. On the Brazilian end, Brazil was in an economic crisis. It was still under a military dictatorship, and they were very short on foreign currency. The then-Brazilian minister of finances, [Antonio] Delfim Netto, who was a well-known economist, thought that they would be able to save foreign currency if they could get some money injected from the World Bank to support certain areas. Chemistry was the area that was proposed initially, because a study by the planning ministry showed that Brazil imported \$12 billion a year of chemicals, whereas the raw materials for producing them were in Brazil, and in principle they could be synthesized in a Brazilian industry. The World Bank thought that that activity was too narrow to be the basis of a loan. World Bank loans are typically on the order of \$100 million a year for three to five years. They suggested that he look into it more

carefully and put a bigger package together. So they—the Brazilians—identified two other areas that were equally in need. Biotechnology because, again, that permitted leapfrogging; you didn't have to go through all of the stages that the first world went through; you could jump right in. And Brazil was rich in biological natural resources. A third area that they identified was mineral technology and geosciences, because it was very rich in ores. What's more, it exported ores and re-imported the materials as manufactured products based on those ores.

COHEN: Brazil's really a very rich country, isn't it?

KUPPERMANN: It has an enormous amount of natural resources. However its main wealth, or an equally important source of wealth, is human brains. It has a very large population, more than half of the population of the United States—160 million—and about twenty percent of Brazil, perhaps more, can be classified as a first world. The southern part, the states of Mina Gerais, São Paulo, Rio and Rio Grande do Sul—I wouldn't be surprised if they contain about forty percent of the population of the country. These are places where the level of education is high, the development is high, and they produce extremely good human resources, but they are not—or were not—utilized to their potential. The Brazilian ministry of planning was trying to fund these people who were starting to come out of Brazilian universities. They had had a previous plan, by which they sent a large number of young Brazilians to get their PhDs in Europe and the United States, and they were returning to these new universities in Brazil, which the same government had developed—thirty new universities in a period of—

COHEN: This was a totalitarian government.

KUPPERMANN: Yes. This totalitarian government saw the need for more universities in Brazil. These young people were coming back, and had no funds to do anything with their knowledge. They couldn't create laboratories or do research; and they recognized it as a serious need. The funding for these areas was considered economically important, because if you developed these three areas—chemistry, geosciences and mineral technology, and biotechnology—that could, in the long range, have a large impact on the Brazilian economy. So they did put together a package that was more comprehensive. Then there were preliminary contacts between the World Bank and Brazil along those lines. At that point, the World Bank realized that they did not have

the in-house expertise to analyze the proposal the Brazilians had submitted and suggest improvements. They started looking around, and they found the history of this cooperative program between the Academy and the Brazilian Research Council. They started tracking people, and they found me. I was very appealing to them, because I was Brazilian, I had a good knowledge of Brazilian conditions, a good knowledge of American conditions, and experience. So they tracked me down and hired me as a consultant in early 1983.

COHEN: That paid for your trip home to see the family. [Laughter]

KUPPERMANN: That's right. [Laughter] I had been going to Brazil every year earlier in the cooperative agreement program, then there was a hiatus, and then it started taking me back to Brazil again about once or twice a year. It became obvious to me immediately, as a scientist, that they had two very severe shortcomings: One of them was that they didn't have a developed peer review system. They had a crony peer review system. To really improve these areas you really had to open them up, the qualifications of the people had to count more than their political connections, and they didn't have that. The second one was one that we had encountered in the cooperative agreement in terms of infrastructure support for science. They didn't have machine shops. They didn't have analytical chemical facilities. They didn't have rapid importation of chemicals that would be needed. If you wanted to do something much bigger than the cooperative agreement had done, you really needed to establish an infrastructure to support it. At my recommendation the areas were expanded from these three areas, which were called vertical, to include several infrastructure areas, which were called horizontal. Those were a maintenance program to train people to be capable of maintaining scientific equipment, a rapid importation program, and an information program, which was the libraries—I mean, they were very poor in library resources. So this became then a much bigger program.

COHEN: How about the cronyism? That seems more difficult.

KUPPERMANN: Yeah. Well, in order to overcome the cronyism problem and the fact that that was a totalitarian regime, we wanted—again, at my recommendation, and the World Bank people were extremely supportive—there was a Princeton-educated economist by the name of Ralph Harbison who was the head of the World Bank loan project for Brazil for this purpose.

We both realized that we had to put the scientific community in charge of running the program. The program was very different from ordinary World Bank loans. Normally they lend you money for building a refinery, building a road—

COHEN: Something you can then look at.

KUPPERMANN: And then, ahead of time, they agree on the design, the project, the firms that will implement it, and there are no decisions—all decisions are made by the time the loan agreement between the bank and the government is signed. It's not a grant, it's a loan. In other words, the government eventually pays back the World Bank at reasonable interest, but it's a long-term payback. With this one you couldn't make a pre-agreement of several thousand research projects in these several areas, so there had to be a lot of decision making by the Brazilians, but the decision-making process had to be of a quality such that if the World Bank itself were involved in these thousands of decisions, they would make decisions similar to those of the Brazilians. So we needed to have a structure that was trustworthy and that structure had to, as a result, involve the people who were going to implement the actual work. They were the end-of-the-line recipients, the scientists themselves. So the Brazilian scientists planned this and established a structure in which each one of the areas would have an evaluation committee, and then there would be an overseeing group, an allocation committee that would allocate the resources as a result of open competition somewhat akin to the National Science Foundation of the United States. Then there would be a supervisory group that would look at the outputs coming in from the research that was being supported, to decide whether it was achieving its goal, whether there should be a redistribution of funding between the areas, and so on. All of these decisions would be made by these committees, which were committees of scientists, and that was a no-no for the Brazilian government. In particular, the head of the Brazilian NSF wouldn't accept it. So there was this issue: Do we go ahead anyhow and let him have control rather than the scientific community, or do we decide that it simply didn't have a fair chance of working and it would be a waste of funding? My World Bank colleague, Ralph Harbison, agreed with me that we should stay put. So we said, "Well, we are sorry if you don't agree to the structure that was recommended by the Brazilian scientific community. With our collective experience in international science, it is done at the first level in first countries"—and that's what the objective

was, to raise the level of education and training in these areas to first-world status. Well, Delfim Netto, the minister of finances, really wanted the \$100 million a year to relieve the situation—not that he would be able to use it for other purposes, but it would decrease pressure on the small amount of foreign resources, foreign currency that Brazil had. So eventually, after a year or a year and a half in limbo, he said, “Okay, we’ll sign this.”

COHEN: So you really introduced democracy to Brazil.

KUPPERMANN: It reinforced their peer review system, modernized it, and eliminated cronyism. It made everything open and transparent. The basic rule was that the rules would be transparent and open to scrutiny and anybody who felt that they were not obeyed would be free to complain, and this is probably the most important product of this World Bank loan. It lasted. The third round of the loan is still underway. Right now it’s sort of in decline, because the current government lost interest in it. But the peer review system that got instituted—or reinforced—the Brazilians get very touchy when I say instituted, because they had one; it simply didn’t work.

COHEN: It’s a little different, okay.

KUPPERMANN: The way it worked before is that the Brazilian Research Council had so little money, and they had such a large number of applicants for that money, that they took the money they had, divided it by the number of applicants, and gave each applicant, by and large, the same amount of money in a narrow range. It meant \$2,000 per year per proposal. These applications were subject to a peer review, but it really was more pro forma. We were speaking of this as another very central issue that this loan introduced, which was the elimination or avoidance of fragmentation of resources. You take ten people and give them \$2,000 per year, or ten or twenty groups and give them \$2,000 or \$3,000. That’s \$60,000. What gets done? Nothing. You say, “Let’s take the same amount of money, \$60,000. Instead of giving it to twenty groups, let’s give it to one group.” What gets done? More than otherwise would have. So we tried to eliminate or ameliorate or attenuate the fragmentation problem, which is a political one. We said, “These, research grants have to be in a certain range of monies,” and they couldn’t be year by year. The previous Brazilian system essentially was that every year these people got their \$2,000 and made a plan for \$2,000. We said we want three- to five-year projects that had a broader scope. It was

difficult to implement the five-year stuff, but the two-year stuff got implemented quickly, then it expanded to three years, and that's okay. So it really had a major impact. The first loan, which started in 1985, I believe—it took two years to negotiate, because of the political democracy, totalitarian thing. It was supposed to last for five years, but the importation difficulties and Brazil's failure to release counterpart funds slowed it down. The loan agreement provided that for every dollar the Bank loaned them, Brazil would contribute one dollar—not in foreign currency but Brazilian—for local expenses. That was more or less the proportion of importation of equipment and foreign services to local expenditures.

COHEN: Was that how the World Bank operated? I mean, was that common?

KUPPERMANN: That was common for everything. Due to the very difficult financial situation Brazil was undergoing at the time, they didn't contribute their part, so the World Bank could not make the loan. In addition, even though all of the importations had a foreign component, there were still very restrictive regulations that slowed them down. Even though the monies were not Brazilian dollars—they were coming from abroad—still the whole process was slow. So the initial five years lasted for eight years, with the same amount of money. It just took the Brazilians that long to spend it. Then, when that was over, it was renewed for a second term. Again it was supposed to be for five years, and again it took seven; so there are fourteen years, and '84 or '85 plus fourteen brings us to '98, '99.

COHEN: So here we are.

KUPPERMANN: Here we are. The third loan is now underway. This third loan was aiming at technology. The first two loans were pure science. I mean, their objective was to train human resources at the first-world level of science. The third one is an attempt to integrate the science and technology, to try to get an interface going between universities and industry in Brazil. Up to the third loan, the previous people involved in Brazil—a Ministry of Science was created, and the first three ministers of science were scientists, it turns out, and two of those three were involved in this project from its inception. There was a biologist. There was a minister of science named [Jose] Vargas, who was a physical chemist, and [Jose] Goldemberg, who was a physicist by training. They realized the importance of this project as being one of the only

sources of money to support science in Brazilian universities. The current minister of science is an outsider, a political appointee, and he hasn't yet acquired the perspective that a scientist would have. As a result, this program is in decline. Once more, the monies aren't being spent. So the Brazilians are coping with getting more monies through their National Science Foundation that doesn't go through these programs, but that does go through the peer review system that was established and strengthened by these programs. So the Brazilians are doing much better than they would have done without this whole project, but they're not in the best of shape because of funding.

COHEN: Are you still involved with this project at all?

KUPPERMANN: No. The World Bank goes down and has periodic missions to evaluate progress, but when the Brazilians don't spend the monies, the World Bank doesn't go down. So I haven't been down to Brazil for about two years now. The project was sufficiently successful on its own merits that it spawned or catalyzed similar projects in other countries—Mexico, Chile, and, most importantly, China.

COHEN: So you've been involved in that?

KUPPERMANN: The China experience was very interesting, because it was very different. The China experience got started at about the same time as the Brazilian one. The first loan to China took place in the early eighties, and it was very specific. It was mainly to help the Chinese re-equip their laboratories after the Cultural Revolution. Due to China's scarce economic resources, they got a big loan of about \$120 million for equipment. That loan wasn't highly peer-reviewed or supervised. They fundamentally put down a list of equipment that they needed all over the country. The World Bank got the Academy of Sciences involved, not to oversee the individual pieces of equipment, but to keep an overall eye that it was scientific equipment that was going to the proper places. As part of that first loan, they had a project of foreign experts who they would hire to come and help get the equipment used, and also to teach—to give a series of courses in areas that had never evolved in China because of the Communist regime, the Cultural Revolution, and their isolation. Purely fortuitously, I was invited at that time—not on the World Bank side but as one of these foreign experts—by a colleague of mine at Shandong

University who wanted modern quantum reaction dynamics to be injected into China. He applied to the World Bank loan funds for funds to invite me, and so I came in as a recipient of funds of that program.

COHEN: I see, on the other end of it.

KUPPERMANN: On the other end of it. I spent two months there and taught a course attended by young assistant professors from all over China; about twenty of them came.

COHEN: And this was in Shandong?

KUPPERMANN: That was at Shandong University. Jinan is the name of the city, the province is Shandong, and the university's name was Shandong. This was the first injection of modern reaction dynamics into China. Well, after that came the second and third World Bank loans. The second World Bank loan was for the creation of what the Chinese called key laboratories. The idea was similar to the Brazilian one. There were key areas that, if they could be funded and developed, would accelerate the Chinese economic development. By that time the World Bank was a little more knowledgeable in matters of science and technology, partly because of the Brazilian experience. The woman at the World Bank in charge of the Chinese loan tracked me down, but now internally, through the fellow who was in charge of the Brazilian project. He suggested me, and they then—

COHEN: But you were already there.

KUPPERMANN: Well, I was a consultant for the bank, but I wasn't an employee of the bank. I advised mainly the Brazilian project. Barbara Searle, who was the woman involved in the Chinese project, then asked me to help them with the Chinese project. I went there for the peer review of the second loan, which was now focused not only on equipment, but also on scientific—

COHEN: Now, this was after you had spent your two months there?

KUPPERMANN: Yeah. This was several years after. I spent my two months there in 1984. This was five years after—1989. So I had some Chinese experience as part of my activities and responsibilities. When I spent my two months there, I had to give an overall assessment of how the equipment was being used, what the structure of that particular university was, and so on. So I became knowledgeable about the structure of that university, how it was organized, and how scientists operated or didn't operate. It was typical of most Chinese universities, so even though it was a single one, it gave me an overview. That experience was useful for the Bank, so I went down there to help evaluate their first batch of peer-reviewed projects. What they had done was pick 120 key laboratories, of which a certain fraction, something on the order of seventy, were owned by or under the supervision of the Chinese Ministry of Science and Technology, and about fifty were university laboratories, so the majority were not university laboratories. So they had 120 projects. They said they had reviewed them with the Chinese internal system and here's what they were. That's when I first went down; I visited as part of a mission, I wasn't the only one. I was initially the only scientist in the group. There were economists and sociologists and so on. I visited the Chinese universities more extensively and then examined these 120 proposals. The ones that belonged to the Ministry—there were about seventy of them—every single one of them was at \$1.2 million for the five-year duration of the project, and every one of the university ones was at \$700,000 for five years. I asked several questions. I mean, the basic rule of the game is that you request the funds based upon the function, so why did all of the laboratories need exactly the same amount of money? The first batch was \$1.2 million, plus or minus \$0.01 million. They said, "Well, that's the way we do things." I said, "No. This is funds in proportion to needs. You can have two laboratories and two ministries, and one wants to do one thing and one wants to do another thing, and they require different equipment, different resources, different everything." So we didn't accept it. My recommendation was not to approve those and to suggest that they reexamine. They did and I went back on another mission six months later, and here were these modified proposals. Well, the distribution function of the Ministry laboratories, instead of one being \$1.2 million plus or minus \$0.01 million was \$1.2 million plus or minus \$0.1 million. We decided that the culture was so different, their experience under the Communist regime was so different, and this egalitarianism where you divide things equally was so embedded, that if we didn't accept that, there was no way they were going to get funding. So we decided that was the lesser of two evils and approved the project,

but with strong recommendations of cooperation between the laboratories, infrastructure arrangements, and strong interaction with the National Science Foundation of China.

COHEN: Was language ever a problem?

KUPPERMANN: No. The negotiations were partly with science administrators and partly with Chinese planners. The meetings were with the Chinese planners, the State Planning Commission, which was a high-level planning agency for the whole country. The people could understand English, not speak it very well, but the meetings were always with translators, and they were lengthy as a result. Everything they said was translated into English, and everything we said was translated into Chinese. That's the way it was done, even when some individuals could speak English. One or two of our people could speak Mandarin. So it slowed things down, but it wasn't a very fundamental problem. It was less pronounced at the laboratories themselves.

COHEN: Let me turn this over now. [**Tape ends**]

Begin Tape 4, Side 2

KUPPERMANN: The net effect was that we helped establish some collective activities which were not these laboratories acting in independence. In other words, the Brazilian experience was useful. One had to do with maintenance; the other had to do with computing. Computing was dismal in China at the time. They only had little PCs, old-fashioned ones, and the whole country operated that way. We suggested and they bought the idea of establishing a big computer center that would service the Beijing area. That was an opportunity to leapfrog by getting a parallel computer. There were strong constraints from the American side—the Department of Commerce—of not allowing advanced computing that had to do with the design of nuclear weapons. That really held the project back. The idea was to have a communal facility. They had an internal competition between universities and the Laboratory for Computing of the Chinese Academy of Sciences. By then Sid Karin, the head of the San Diego Super Computer Center who I had recommended be hired as an advisor, was involved, and we had very good

expertise. The World Bank mission thought that the Beijing University proposal was the strongest one, but the Chinese approved the State Key Laboratory of Scientific/Engineering Computing of the Chinese Academy of Sciences to be the place.

COHEN: Now, Aron, how much of your time did this use up? I mean, you were still running your whole research program here. It sounds like an overwhelming more than full-time job.

KUPPERMANN: Yeah. But it was integrated over almost fifteen years, so it never took more than five percent of my time per year, and it was usually two percent of my time. In other words, it was essentially on the order of three or four weeks per year, at most.

COHEN: You would go off. So you really should know China quite well.

KUPPERMANN: Yeah. I went to China three or four times as part of the oversight missions, and so on, but it never really cut into my real time. We're entitled as Caltech faculty to one day a week, and it never exceeded that.

COHEN: So is that mission sort of completed now?

KUPPERMANN: Yeah. Well, I was finishing the story on the parallel computing. The Chinese Academy of Sciences got that parallel computer and never let anybody else use it. [Laughter] However, because of the activity stimulated by it, the Beijing University people who had their own proposal were able to raise funds from other sources and get a second one that is still serving the community. So again, once you get a foot in the door and eliminate the central authority, and the community gets involved, then you cannot maintain the old system, because it really requires a closed system. Any open system evolves naturally into the first-world system because that's the one that has been proven by sociological development, natural evolution, and so on.

COHEN: So it really changes the culture.

KUPPERMANN: It did change. Their science foundation became much stricter in their peer review and they have a very good peer review system there. They have this parallel computer, and they have an open policy, and so it has had an impact. Up to the end of the second project, which was about four years ago, the Chinese had been getting very favorable loans which were more like grants—they had to pay very, very little; two or three percent a year. By then they had developed economically, and in applying for a third loan they wanted the same kind of ultra-favorable treatment that is given to poor African countries. The World Bank said, “No. Come on now. You’re developed. Now you have to pay the same rate as Mexico and Brazil. You’re not worse off.” The Chinese said, “Well, those are commercial rates for those who don’t need your help. Thank you.” So they did not apply for a third loan. What they get with these loans is expertise from abroad, but the Chinese are very proud, and they feel that they know better, generally speaking—I mean the government, not the scientists. The government felt that if they were going to go to the commercial market, they could do it on their own; they didn’t need this World Bank expertise. So that was the end of it. My last trip was a final assessment. That was in ’97 or ’98. I took Roza with me, and that was good, because I didn’t know that that was going to be the end of it, but it was. So the Chinese activity of the World Bank has ended by now, but it lasted from ’84 to ’98, so fifteen years.

COHEN: That’s a long time. So are you doing anything with the World Bank anymore?

KUPPERMANN: Yeah. There’s a Mexican program going on, which has been going on also for over ten years. It started five years after the Brazilian one. I was in a supervision mission, which is World Bank jargon, a year ago last June, and that went fine. Since then there was a change in government. In a Latin country, whenever there’s a change in government it affects everything. This program is run internally in Mexico, by the Mexican National Council for Science and Technology called the CONACyT, and they have a new chairman and a new structure, and so they have not yet scheduled the new supervision mission, which was due in June—it’s once a year.

COHEN: I’m thinking, “Well, Bush loves the Mexicans so much.”

KUPPERMANN: Yeah. So right now the Mexico activity is the active one, but it's in a transition period.

COHEN: Well, it's not such a long air flight. [Laughter] So that's really fairly interesting. Do you do any other professional activities with the chemists?

KUPPERMANN: Yes. I'll go into that, but I want to close up the World Bank experience in terms of a language issue. When I was lecturing in China for a month and a half—and then traveled for half a month—this was going to be a large number of lectures; about forty hours of lecturing, so I asked my host whether there would be a simultaneous translation. He said, “Oh, no, no. They understand English quite well. These are scientists.” Fine. So the first lecture was a standard three-hour type in English, and at the end I asked, “Are there any questions?” and there weren't. I didn't expect any. These were young assistant professors breaking the ice who didn't feel comfortable displaying ignorance by asking questions. I said, “Well, either I am a perfect lecturer or you are perfect students to have no questions.” There wasn't a single smile, and I knew I was in trouble. So I took out a textbook that I had brought with me, opened it, and gave it to somebody in the front row and asked him to read a paragraph, which he did. I couldn't understand a single word of what he was reading, but it was obvious that his colleagues did understand him. It turns out that they were indeed fluent in written English. They were even fluent in spoken English, but their spoken English had nothing to do with our spoken English. I dug into that later and I found out that many of them had learned English from people who were originally Russian instructors. When China broke with Russia, they converted these Russian-language Chinese instructors into English-language Chinese instructors. They didn't know English, so they did the best they could, and then they trained others. In 1984 there was very little traffic of English-speaking people in China. Right after the Cultural Revolution China was still isolated. So there simply was no such thing as a Chinese understanding of spoken English. When I found that out, I had to then write all of my lectures on overheads. To deliver a three-hour lecture took me ten hours of writing. From then on, I would project these overheads. I had a pointer and I read them aloud. I didn't say any word that wasn't written. After about half of the series of lectures, they started understanding my spoken English, because they could see the written one and they could hear my spoken one. I don't know how much quantum reaction

dynamics they learned. There was no exam, of course. [Laughter] I think that they learned some Brazilian-accented English. So that was a very interesting experience, and it was a very good—

COHEN: It sounds like a lot of work.

KUPPERMANN: It was. I would spend the night writing these ten hours, then deliver the lecture the next day, and then come back to the apartment. Writing and lecturing and sleeping consumed almost all my time.

COHEN: A labor of love.

KUPPERMANN: Anyhow, that sort of closes the World Bank experience.

COHEN: But you're still involved in Mexico. So you really think the World Bank is a good organization.

KUPPERMANN: Yes, I really think they have been.

COHEN: Where are their offices?

KUPPERMANN: In Washington. Their objective, of course, is to accelerate the economic development of the third world and eliminate poverty in the world. Their staff is mainly made up of economists, engineers, and sociologists. They sort of have an internal division. They divide themselves between people involved in operations, which are the people who go on these missions, examining and developing the loans, and then there's the internal studies' group.

COHEN: I remember Bob Oliver went and worked for them for a couple years.

KUPPERMANN: That's right. The people who do the very hard work are the people who do the fieldwork. As a result, they don't get too involved in the internal politics of the other group, and it's the other group that runs the World Bank. If they were reviewed from the point of view of a

rational structure, an organization—the way they review the loan applicants in terms of rationality and achieving objectives—they would fail a World Bank-type of scrutiny.

COHEN: But they seem to accomplish a great deal.

KUPPERMANN: Yeah, they do.

COHEN: So your own chemistry.

KUPPERMANN: In terms of activities of a chemical nature outside of my research, in addition to this World Bank thing, my main activity currently is in the National Science Foundation. Well, right now it's called the National Partnership for Advanced Computational Infrastructure, which is a descendent of the National Science Foundation Centers. I am a member of the executive board. There are only two of those. There's the so-called NPACI, which is the acronym for the National Partnership for Advanced Computational Infrastructure. The other one is centered in Illinois, NCSA—the National Center for Supercomputing Applications. These two groups have all the NSF funds for advanced computing in the country that is open to general use. The Department of Energy has one, but they are limited to Department of Energy applications, some of which are classified. So I am on this San Diego one, the head of their users committee that is supposed to get input from all of the scientists in the country using that particular center, and I'm a member of their executive board. Right now we're in an important phase of transition, because this is the first five-year period since the National Science Foundation Centers' project was transformed into this national infrastructure program. They are being reviewed for a second five-year project. In addition, there is a new distributed teraflop initiative involving a loan of something on the order of \$40 million to upgrade these two centers to be state of the art, which they are not. This distributed teraflop project—

COHEN: Tera?

KUPPERMANN: Teraflop. Remember, mega is million; it's ten to the sixth. Giga is a billion; it's ten to the ninth. The next one is tera, which is ten to the twelfth; so it means ten to the twelfth floating operations per second. That's what the word teraflop means.

COHEN: I see. So this is a technical term.

KUPPERMANN: It's a technical term that indicates the speed or the power of the computer. This teraflop computer is distributed because parts of the equipment will be located in San Diego, parts in Urbana, Illinois, and even a piece of the action will be at Caltech, which will have a half of a teraflop.

COHEN: Okay. Each one of these things has its own vocabulary.

KUPPERMANN: That's right. Yeah. I apologize.

COHEN: So how much of your time does this take up?

KUPPERMANN: We meet four times a year for two days—the next meeting is in early November—and then I have a users' group meeting. So the activity is something like ten, twelve days a year.

COHEN: So you have a finger in the international scene, a finger in the national scene, and of course here where you live. It sounds like a lot of full-time jobs. So anyway, Aron, let's talk about what you think about Caltech. Do you like being here?

KUPPERMANN: Yeah, I love being here. Caltech is a wonderful place. As you remarked previously, other than Millikan, I have worked under every president Caltech has had. Of course the first one when I came here was Lee DuBridge. Linus Pauling was still here when I was offered the position, but he was already emeritus. Feynman was here. I had met Feynman when he visited Brazil.

COHEN: Ah, when he learned to play his drums.

KUPPERMANN: That's right. He visited the Institute for Aeronautical Engineering, where I was a young faculty member. That's when I first met him. So when I was being interviewed, I spoke with Feynman, I spoke with DuBridge, I explained the nature of my research, and so on. Soon

after I came here there was some activity of the board of trustees. There was a joint dinner or something between the board of trustees and the faculty, and I was in the Athenaeum at a table.

COHEN: That would have been about 1965?

KUPPERMANN: Probably, or '64. I came in '63, the end of the summer of '63. This must have been late '63 or early '64. We were at the table in the Athenaeum, and this member of the board of trustees asked me what I did, what my research was, and before I could answer, DuBridge told this member of the board of trustees what my research was. That was absolutely spectacular. It impressed me enormously. DuBridge was always very helpful and very interesting, and I enjoyed him very much. The chairman of the board of trustees was Arnold Beckman. Well, Arnold Beckman is an old University of Illinois alumnus, and when he found out that I came from there, he immediately was interested and we chatted. Then some of my research, the part that popped up in that book by Mitchell Wilson [*Passion to Know*, 1972]—about the reaction of a mono in a single-energy deuterium atom—came out in *Time Magazine*—a news item came out on that. I gave a lecture to the board of trustees about that, and Arnold Beckman was present and said he'd like to talk about it. We considered each other fellow alumni. There was a very good bond between us. That made my interaction both with the president and with the board of trustees very, very pleasant, and I enjoyed it very much. After DuBridge was appointed by President Nixon as science advisor, he was replaced by Harold Brown. Harold Brown was a physicist by training but soon after getting his degree he went to—I believe it was—Livermore.

COHEN: Right. So he was an administrator very early on.

KUPPERMANN: Then he came to Caltech. Beckman knew him from his activities. He was Secretary of the Air Force, if I remember correctly, before coming to Caltech. I was initially a little concerned, but then soon after he came I organized a meeting at Caltech on reaction dynamics and industrial associates, and I asked him to come do the introductory remarks. He said there that it was sort of interesting for him, because, as a result of what [Paul Adrien Maurice] Dirac had said in the early days of quantum mechanics, he didn't think that there was much need for this research, since we could compute it all. He said this facetiously, of course. Later on, as we accidentally were walking towards the Athenaeum side by side on another day, I

told him, “You know, Harold, you said it facetiously, but it’s not totally facetious. There has been major progress along those lines, and particularly what I do is an attempt to achieve that, to replace experiments by calculations.” He said, “I would like to hear more about it.” So I said, “Why don’t you come visit my labs?” He said, “Okay, I will.” The next day, I got a call from his secretary, and within a few days he shows up in the lab and we talked about science, what I was doing, and so on. That was, again, very impressive, because even though he was a science administrator, he still had a fundamental interest in science. He was interested enough to come and try to understand what one of the faculty at Caltech was doing. So I thought that Harold Brown, generally speaking, also did very well, in spite of my initial concerns.

COHEN: Being a military person?

KUPPERMANN: When he left to become Secretary of Defense in the Carter administration—

COHEN: I think [Robert] Christy was acting [president] for a while.

KUPPERMANN: Yes, Christy was acting for a few months, and then the permanent one was Murph Goldberger. Murph was a different type of person than Harold Brown. Harold Brown was very logical, intellectually organized. Murph was a very bright person, but in addition he was a people person. Harold Brown didn’t interact easily with other people, including the board of trustees. He got along well with them because he ran the institute well and kept the finances under control. Murph was more of an interactive person. It was during Murph’s regime that parallel computing at Caltech was flourishing. Robbie Vogt as a provost appointed a committee to look into computational needs. As I mentioned before—

COHEN: Yeah, we already talked about it. He was quite sympathetic to it.

KUPPERMANN: That’s right. As I think I mentioned, the parallel computing activity at Caltech—this committee that I chaired—was going to be funded by Murph, but before any decisions were made—

COHEN: [Laughter] Yeah, you did mention it, that [Thomas E.] Everhart came and was not sympathetic to it.

KUPPERMANN: Everhart was interested, and I sent him a copy of this report. He read it, but he fundamentally felt that computing should pay for itself. The National Science Foundation had changed its policies. Whereas previously every researcher could put down in his research grant so many hours of computer time, and that's the money that went to pay for computing time, that was no longer true. The whole economics of computing changed. It was important to get hardware from NSF, but to get hardware you always needed a matching grant from—

COHEN: Your institution?

KUPPERMANN: Yes. So the idea of having a zero cost without significant involvement was and is not really viable. I felt personally that Everhart was too cautious. He missed opportunities by allowing very exciting, competent faculty to go because they needed more help from the institute than Everhart was willing to give. Lee Hood left, and others in biology left—several people. There was this new Center for Advanced Computing Research that we wanted to get started, but that would require funding, and that funding was really very limited. So I felt personally that although Everhart was a sound individual, he was too cautious, and that caution, from my perspective, was excessive.

COHEN: Well, now we have a new president. I think he has a lot of vision, probably.

KUPPERMANN: Now we have a new president [David Baltimore] who has a lot of vision, and we'll see what will happen. In terms of computing, he is playing a less active role and is leaving it more to the provost, and the provost has inherited the Everhart perspective: it should be done, but the institute should not have to make a significant contribution. There's a certain amount of funding coming to the Center for Advanced Computing Research, but from my perspective it's not enough to make the activity viable. So far we have been able to survive, through these different National Science Foundation and Department of Energy initiatives, but the problem has not yet been resolved long range. For two or three years it has sort of been moving along.

COHEN: But I would say you've mostly had a good time.

KUPPERMANN: I've had a wonderful time at Caltech. It's a wonderful institution. I've enjoyed my entire time here, and continue to enjoy it while it lasts.

COHEN: Yes, of course. Is there anything else you want to add?

KUPPERMANN: No. Thank you very much for listening to me. **[Tape ends]**

ARON KUPPERMANN

SESSION 5

November 15, 2001

Begin Tape 5, Side 1

COHEN: Good afternoon, Aron.

KUPPERMANN: Good afternoon.

COHEN: It's November 15th, 2001. We're going to revisit several things. One of them is your involvement in the community.

KUPPERMANN: Sure. When we first moved to Pasadena, one of our first activities, of course, was to look for a house, which we did, and within six months we bought one. We found that at the time there were in the documents restrictive conditions on the purchase of property in the Pasadena/Altadena area that went under the name of "conditions, covenants, and constraints"—the three Cs. I found out that one of those was that you were not permitted to sell properties to Chinese, and perhaps to Japanese also.

COHEN: I think there would have been more of a concern about Japanese at that time.

KUPPERMANN: Yeah, it could be. But, no, the conditions were instituted before World War II, in the tens and twenties. I think that there were many Chinese laborers, and they were concerned about that. I consulted with the Caltech lawyers at the time, because I didn't want to sign a piece of paper that was discriminatory, and I found out that those conditions had no legal validity anymore. They had been declared unconstitutional, and even though they were in the documents, they were devoid of validity. That called my attention to the issues of buying property and of housing. In particular, northwest Altadena was among the places we looked at in the beginning, where there were very nice properties. It was a partly mixed neighborhood, with blacks living there, and we were told by realtors at the time that we would have a very difficult time obtaining financing to buy property there, because they did not like the idea of mixed

neighborhoods. Similarly, when a black family wanted to buy property—like a house for residential housing—on the east side of Lake Avenue, they would have equal difficulty in, number one, finding financing, and, number two, finding a realtor willing to help them negotiate such a property. Roza and I were very upset about that. There were other Caltech faculty who were also upset, so we got together and founded an association called Housing Information Service to help black people who wanted to and could afford to buy property anywhere they wanted to find the means of doing so.

COHEN: Who else was involved with this?

KUPPERMANN: Well, there was Bill [William J.] Dreyer. Bill and Mary Dreyer were involved. I don't remember the rest of the faculty. I remember that Jim [James] and Peggy Knecht were involved. He was a lawyer in town and she was a nurse, but they were not Caltech people. They were Caltech Associates, or have since become Caltech Associates. There were some black professionals involved, lawyers and physicians—blacks who were generally speaking reasonably well to do, had made it out of the ghetto, and were hampered by these restrictions. That organization acted for a few years, during which the social barriers slowly broke down.

COHEN: We're talking about the late sixties?

KUPPERMANN: Yes. We're talking about the period from about '65 to '68 or '69. By then these constraints were loosened and people, blacks, were able to find property and funding and so on. So the need for the organization significantly decreased, and the association died, since it was no longer needed. At the time I felt it was something that was useful and important.

COHEN: And you really helped several people go through this maze of buying houses?

KUPPERMANN: We helped direct them to realtors—the small number of realtors—who were willing to do that. We were able to direct them to lawyers who could help them, because all of these constraints were totally illegal. I don't know how many people we helped directly, but the sociology of the time was such that, for whatever reason, it did work. We were probably just one

small element of the whole picture. So that was a community activity involving some Caltech people but involving mainly the sociology of the community.

The second type of communal activity that I was involved in was becoming a member of the Pasadena Educational Foundation, which is an association of private individuals whose objective is to try to improve and help primary and secondary public education in the area through whatever means necessary. I became a member of that group through my activities on Caltech's Committee for Relations with the Community. They wanted broader involvement in that foundation, and because Caltech was involved in education, it was a natural fit.

COHEN: Were you encouraged by administrators here at Caltech to do this?

KUPPERMANN: To the best of my recollection, I had their tacit approval. There was neither strong encouragement nor discouragement. We realized that for Caltech to be an attractive institution for good faculty, there had to be a good public education structure. In those years it was still not that common for people to send their children to private schools—although there were some, many, many faculty members sent them to public schools. The public schools were decreasing in quality, partly because of the large influx of minorities without an influx of a concomitant amount of funding necessary to attend to the needs of a changing student population. In that Pasadena Education Foundation we discussed—through me Caltech got involved in several things, including pilot programs for bringing some of Caltech's educational expertise to the public schools through courses for teachers during the summer. At the time there was increased Caltech activity in summer programs at Caltech proper, inviting students from the area to come and take summer courses organized at Caltech on a volunteer basis. Lee Browne joined Caltech a little bit later, after these activities with the Pasadena Education Foundation, but not totally unrelated to them.

COHEN: That was the beginning of it.

KUPPERMANN: The beginning of this type of thing.

COHEN: Now, was Harold Brown still here at that time?

KUPPERMANN: Yes. He was still here, because Harold Brown was here from '69 until Jimmy Carter took office in '75. If my memory serves me right, this was still during that period. I consider that to have been a useful—

COHEN: How much of your time did you give to this?

KUPPERMANN: Oh, the amount of time was not very extensive. There were two kinds of time: meeting time, and we met perhaps once every week or two, and work behind the scenes time, talking with people and getting people interested and involved. There was still a residue of this until recently. That was when Jerry [Jerome] Pine got initially involved, and so it was picking up from thirty years ago. Off and on he has kept his own involvement. There was a more recent resurgence of this involving him and Jim Bower and so on.

COHEN: Well, of course, he runs a very big program.

KUPPERMANN: That's right.

COHEN: I mean, maybe not completely sanctioned by Caltech, but anyway—

KUPPERMANN: Yeah. Well, he has left Caltech now.

COHEN: Bower, not Pine.

KUPPERMANN: No, not Pine—but the kernel, the roots of it were from about that period of time.

COHEN: So that was a period of time when the Caltech administration really liked or wanted that sort of thing. I'm not sure if that continued.

KUPPERMANN: No. In addition, as another component of the same Committee for Relations with the Community, which led to the involvement in the Pasadena Educational Foundation, there was also involvement in the quality of Caltech's environment. The University of Chicago was facing difficulties with the deterioration of the neighborhood surrounding it, and they had to take

heroic measures to try to change and improve that. There was a view that Caltech should do something to protect its surroundings against such decay, because it would be much more difficult to reverse after it had set in than to keep it from happening. So at that time we were trying to implement measures with Caltech's involvement that would keep the environment sound. It was then that we started this Committee for Relations with the Community, and the administration and city government starting having joint meetings with the mayor, again in the early seventies. That was when Jim Black [Director of Public Relations] was in the administration. He was involved on the administration's side in relations with the community, so he was the administration person. There was a faculty group that I headed. So we had people from the administration, the faculty, and the city meeting periodically at the Athenaeum and discussing measures and cooperative ventures to keep the sociological environment of the city from deteriorating, since it had started deteriorating. Some of the educational plans and cooperative plans for courses with the public schools and so on evolved from that.

COHEN: How long did that go on, Aron?

KUPPERMANN: It went on for four or five years.

COHEN: Do you think that was because Harold Brown was interested in it?

KUPPERMANN: Partly it was that, and partly it was because the sociology was changing. That was a time when the schools that had been well balanced in terms of ethnic composition, that reflected the ethnic composition of the city, started shifting. The ethnic composition of the public schools started becoming very, very different from the ethnic composition of the city since white flight was occurring in an almost unstoppable way. That change made the overall community, including Caltech—not only Caltech—become concerned with this sociological phenomenon.

COHEN: Of course, don't forget the 210 freeway. It took out, what, 400 houses? Those people left Pasadena.

KUPPERMANN: That is correct. However, the people who left Pasadena, and hence the Pasadena public schools, did not really have an impact on this sociological change in the public schools that, within a period of five years, changed from having an ethnic representation very close to that of the community to essentially a very small white component. The majority of those fled, and these were not people who had fled because of this question of the freeway. The freeway affected perhaps more black neighborhoods than—

COHEN: This was a lower middle-class white community, many of them, who relocated out of Pasadena.

KUPPERMANN: That's correct. In addition to that, and especially in the big area where the 210 crossed the center of town, there was a big black population. I'm not sure that the mixture of white to black was significantly different from that of the composition of the city at large, so I don't think that affected this swing. The swing in the student population is known, and also it's a logical phenomenon. It's like an S-shaped curve, that once it starts, it completes itself. No community in the country has found a way of interrupting it or stopping it once it sets in. Those were the years in which it had set in, and we were trying to stop it, but we were not successful. Then, once that re-equilibrated, I think that the community focused on other concerns.

COHEN: But you did spend time during those years working on that.

KUPPERMANN: Yeah. I remember addressing public meetings in the court, in the square outside of City Hall. There were public gatherings and discussions of the importance of the schools. There were many organizations in town involved, and Caltech was represented in those activities through this Committee for Relations with the Community.

COHEN: But that really ceased by the end of the seventies. As you said, it was irrevocable.

KUPPERMANN: That's right.

COHEN: So that was a good effort while it lasted.

KUPPERMANN: Yeah. A third type of community involvement or activity that I was involved in, and still am, is Villa Esperanza. We have a daughter who has Down syndrome. She was born thirty-five years ago. When she was born we looked around to see what was available in the community to help people in our situation, and there was a very small fledgling association called Villa Esperanza. It was only then realized that Down syndrome was a genetic disease, and that it affected about one percent of the births in the country nationwide. Down children traditionally had been kept either at home or, in more recent years, sent to institutions or hospitals. The Lanterman Center in this area was one of those hospitals. They were not part of the community; they were isolated from the community. However, it was realized that this was a genetic disease that was prevalent to that level, and that something had to be done about it. A woman psychologist in Pasadena—her name is Florence Diamond—founded an infant center in this Villa Esperanza to start trying to educate Down children from the earliest possible time. She felt, and others did also, that even though it was a genetic disease there was a strong component of nurture, and if you started early in the game you could improve the quality of life of Down children.

COHEN: Did she have a Down syndrome child herself?

KUPPERMANN: Not to the best of my knowledge. She founded the center with her money with this association of parents of children with mental disabilities called Villa Esperanza. That was in about 1963 or '64. We discovered this group and we placed Sharon there. It was a day school, a few hours every day, with specialized teachers. We found that to be very useful and very helpful. I got involved in helping the organization, and within a small amount of time I became a member of the board of directors, which I stayed on for almost thirty years. I'm now emeritus of that board, but I'm still involved as a member of the board of the residential facility associated with them, which is funded by HUD, the U.S. Department of Housing and Urban Development. I'm the HUD representative on the board of Villa Esperanza. It's been an association that has lasted for over thirty years and is still going on. Villa Esperanza was small, made up of very devoted teachers and a very devoted director, Elene Chaffee, who I believe was principal of Wilson Elementary School before she joined. She's still alive. She's about one hundred now. She was taken away from retirement to become director of Villa Esperanza, and

she was already in her sixties then, and she stayed on in that capacity for twenty more years and did a superb job. The institution grew to include elementary school classes and high school classes, but then the state government and the state legislature approved laws that made special education a part of the public schools. Some of the programs that had started at Villa were absorbed into the public schools, mainly at Roosevelt School in Pasadena. So some of these programs shrunk. There were still a small number of children for whom the public school environment and the idea of mainstreaming didn't work. Mainstreaming works best if the child or student has a certain level of ability, but below that level, mainstreaming doesn't help. We kept the children who, for whatever reason, were not considered suitable candidates for mainstreaming.

COHEN: So it wasn't only Down syndrome that you dealt with there.

KUPPERMANN: No, but it was mainly Down syndrome. Down syndrome children represented a very large fraction of these children with disabilities. In addition, it was a relatively small group, and we were interested in developing pilot programs that could be replicated elsewhere. We never intended—it was like Caltech in a certain sense—we never intended to serve all the needs of all the people with mental handicaps, because that would have been beyond our abilities as a small volunteer group. So it focused its attention on Down syndrome, but in more recent years it has extended that to autistic children. Right now it's a combination of Down and autistic children who are the majority of the activities, or the clients.

COHEN: Now, Aron, was this strictly a personal thing? Caltech had nothing to do with it?

KUPPERMANN: I did get Caltech indirectly involved. Bill Corcoran, who was vice president for Institute Relations at Caltech, was a friend, and he agreed to serve on the board of Villa, so he was elected to that. He functioned as a very important member of the board of Villa during about five or six years, essentially until his death. So although this was not an official connection with Caltech, it was an unofficial one.

COHEN: It was sort of sanctioned by Caltech?

KUPPERMANN: It was sanctioned by Caltech. He helped guide the finance committee to run in a sounder way, rather than with budget deficits every year, and making those up as emergencies every year to make the payroll. I was involved, starting from when I was still a member of the Committee for Relations with the Community. So this was extra official, but the administration was aware of it and very frequently we had fundraisers for Villa Esperanza at the Athenaeum, sponsored by either Bill or myself. There was an awareness that this was for the good of the community, which it was. So this institution grew. Although at the time, thirty years ago, it was one of the very few institutions or associations of this kind in the country, they are now prevalent because it's since been nationally realized that this is not just a problem of a local community, or even of a negligibly small fraction. One percent is a small fraction, but it's not a negligibly small fraction. If you take a community like Pasadena, a general area that has, let's say, 200,000 people, and include some of the immediate neighborhoods, if you say that—

COHEN: One percent is still quite a bit.

KUPPERMANN: Yeah. So that is an activity that over the years started getting more and more help from the State of California as the problem was understood to be nationwide, but it is still run with a major communal effort of the board of directors, our leaders, and the business and professional community. The programs adapt, and they constitute essentially a lobbying group at the state legislature when legislation comes up that affects the state's involvement with people with disabilities. For a number of years, [Kathryn] Katie Nack, who became mayor of Pasadena—she has a daughter who is a resident of Villa Esperanza, in the same house as our daughter, actually—and she's been very involved. This is just an indication of the fact that, although it's a small group, it is representative of a broad cross-section of the community, and represents a very important pilot activity that has replicated itself, and has had an impact on the way other groups of this ilk are run and the kinds of programs that they offer. As the years have gone by, its programs have adapted to the aging population of Down syndrome, because health concerns with Down children have led to preventive measures that lets them have a life span that is not much shorter than normal people. It means that, for the first time, we have an aging population of grown-up, adult Down. The oldest member—or client—of Villa Esperanza is sixty-two years old now. So the need to develop programs for the elderly mentally handicapped

has evolved, and Villa has taken an active role, and that impacts the community. Although my own involvement came about because of personal conditions, generally speaking it is a communal activity. Since Caltech is part of the same community as Villa Esperanza, there's a synergy.

COHEN: But, Aron, do you see any of the young people now who are so pressured with careers involving themselves in any of these kinds of activities?

KUPPERMANN: I can only speak of my own personal awareness of young Caltech faculty, which is with those in my own department, because I have very little contact now with young faculty throughout the institute. So I have to limit myself to my own department.

COHEN: Chemistry has a big faculty here. They hardly seem social with each other.

KUPPERMANN: That's right. The sociology of the institute has changed enormously over those thirty years for several reasons. Most of the reasons are common to the society at large. Fewer women worked in nine-to-five jobs in those years. As a result, there was much more social interaction among the faculty through dinners and parties and so on. The faculty was more intimately interwoven. That is no longer the case. As you well know, we get together at parties, but the parties are sponsored by Caltech rather than as the result of social interweaving.

COHEN: So that would extend to relations with the community, too, then.

KUPPERMANN: That's right. We've become at Caltech much more—self-centered is not the right word—

COHEN: Self-contained.

KUPPERMANN: Self-contained is a better word, or self-involved. Caltech is no different than anybody else, but I think it does manifest itself through a smaller involvement in social concerns by the young faculty with whom I am familiar.

COHEN: So that's really a great change from that generation to this generation, which is too bad.

KUPPERMANN: Yeah.

COHEN: Okay, Aron. You also wanted to talk a little bit about some of your graduate students.

KUPPERMANN: Yes, that is correct. One of the things that attracted me to Caltech was the potential quality of the students. When I left the University of Illinois, I had no complaints. I didn't leave because of repulsive forces between Urbana and me; I left because of attractive forces between Caltech and me. An important attractive force was that I was aware that the quality of the students at Caltech was higher than that at Illinois. The best Illinois students and the best Caltech students, as I think I may have mentioned earlier, are equally good, but the fraction of the students who are very good on an absolute scale is much higher here. Indeed, when I came here I found that to be the case. I have had the luck, the happiness, over the years of having been able to cooperate with, and partly train, a bunch of very good students, some of whom have really become leaders in the field. The field of quantum reaction dynamics that I discussed earlier was developed over the last thirty years by a relatively small number of groups, one of which is ours, and three of my ex-students are national leaders in the field. In order of decreasing age, one is Don [Donald G.] Truhlar, who is a professor at the University of Minnesota, a national figure in the field, and editor of the *Journal of the American Chemical Society*. He is really an extraordinary individual. He's a very prolific scientist. I have lost track of the number of publications he has, but I believe it's more than 500, probably approaching 1,000. His thesis was a bound volume of about 1,000 pages, and he had about 2,000 references in those pages. Now, having a large number of references in papers is not that difficult, but as a graduate student Don had read all of those 2,000 references and, even more impressive than that, he remembered the contents of every single one of them. When I wrote to the University of Minnesota recommending him for a position on the faculty, I wrote that in my opinion it was quite conceivable that he was a genius. That was in a letter to Bob [Robert] Hexter, who was then chairman of the department of chemistry at Minnesota. Years later, when Hexter retired, he cleaned up his files, and he found that letter I had sent him, and he attached a note saying that I was mistaken, because it wasn't probable that Truhlar was a genius, he really was a genius. [Laughter] Truhlar came from a small college in Minnesota; I believe it was called Saint Olaf

College. He almost was not accepted as a graduate student at Caltech, because, according to some of his letters of recommendation, he had the reputation of being a rebel. Fortunately, we didn't pay much attention to it.

A second one is George Schatz, a professor at Northwestern. All of these three people are international figures. George is the editor of the *Journal of Physical Chemistry*, and really an extraordinary scientist. He has probably co-authored papers with the entire community of people in his field. He is a very, very nice person. He came here as an undergraduate from Clarkson University, again a relatively small place. That's been my experience over the years; that some of our best students didn't come from the big-name universities but from some obscure place where they were the best they ever had, and they never knew how good they would be when matched against the rest.

COHEN: That's probably not true anymore, though. They're not coming from these little schools anymore.

KUPPERMANN: Probably not. That's right, because the high school population is more sophisticated, so this lone soul who kind of drifts into a small college because he doesn't know better—that phenomenon doesn't exist.

COHEN: So who is the third one?

KUPPERMANN: The third one is Joel Bowman. He came to Caltech from Berkeley. Of these three, he was the only to come from a big-name school. He is a professor at Emory University. Again, he is an international figure in his field, and very prolific. Whenever people want to say something nice about me in public, they say that my most important contribution was having trained these three people. [Laughter]

COHEN: Well, okay. Now, these people were all active in this event for you, this birthday?

KUPPERMANN: Yes. As a matter of fact, the three of them, plus a fourth one, Jack Kaye, who again came from a small, well maybe not so small—in New York State, on the Atlantic coast—it's a university that starts with a "D," but it's not very well known. The name that comes to

mind is Dreyfuss, but it's not Dreyfuss. [Jack A. Kaye holds a BS degree from Adelphi University. —*Ed.*]

COHEN: Dixon?

KUPPERMANN: Perhaps. He was also very good. He is now a high-level administrator at NASA, the manager for space science support of NASA, meaning that he is the one who distributes, if you will, the money for science. When somebody at Caltech wants a grant from NASA, they submit proposals to NASA as a funding agency, and he is involved in that. He has a high position in the funding of universities.

COHEN: What is interesting here, Aron, is that you obviously had a strong group all the time you were here, and you still do, but it didn't stop you from taking your leaves or going on your sabbaticals. Many people don't do that.

KUPPERMANN: That's right. That's another point. But let me just finish this. I mentioned that all four of these people are the ones who organized my birthday festivities.

I have taken sabbaticals on average, as the name implies, every seven years. While I was away I usually came back to make sure that everything was all right with the group. I found that my absence did not have a long-lasting deleterious effect. At times it would slow things down a little, but most of the time it didn't. They did as well in my absence as in my presence.

COHEN: [Laughter]

KUPPERMANN: I felt that these sabbaticals were very useful, because most of my new directions in research came from when I was away and could sit back and think. The important point, from my point of view, is that you don't take a sabbatical to get research done, because the best place in the world for you to do the research you're interested in is in your own laboratory. You take a sabbatical from the professional point of view to have the time and the opportunity to think about different areas of scientific activity, different problems. I found that to be true. It also broadens one's perspective of the nature of the world academic community. I found it very useful to take a sabbatical every seven years.

COHEN: That's not a general philosophy around Caltech.

KUPPERMANN: No. The majority of Caltech people, to the best of my knowledge, simply don't take sabbaticals.

COHEN: Okay. Is there anything else?

KUPPERMANN: Nothing. [Laughter]

COHEN: Nothing. Okay. Well, this was a very good addition.

KUPPERMANN: This was a long ten minutes. [Laughter] [**Tape ends**]