



Marshall Fixman

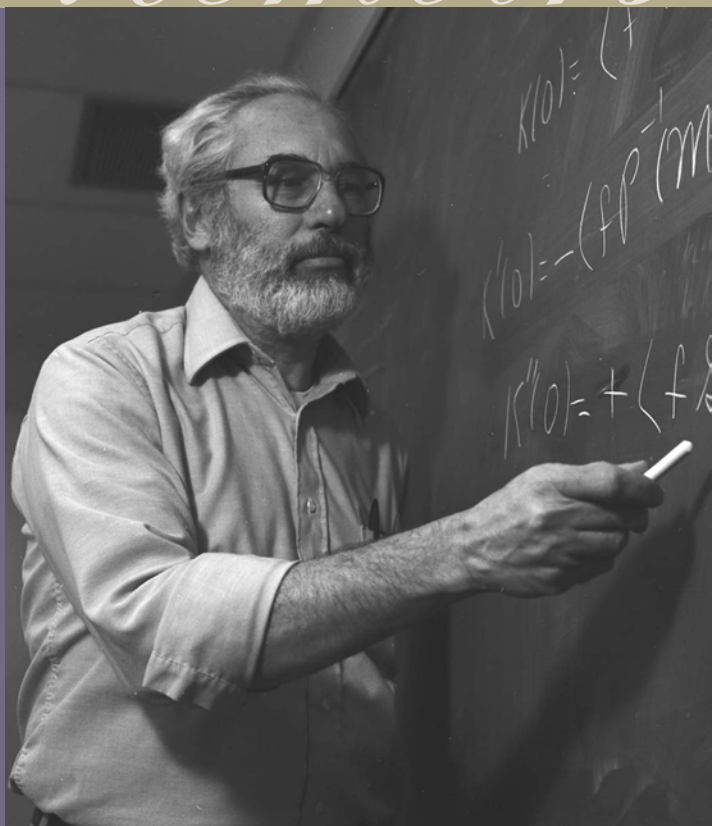
1930–2016

BIOGRAPHICAL

Memiors

*A Biographical Memoir by
Jeffrey Kovac*

©2018 National Academy of Sciences.
Any opinions expressed in this memoir are
those of the author and do not
necessarily reflect the views of the
National Academy of Sciences.



NATIONAL ACADEMY OF SCIENCES

MARSHALL FIXMAN

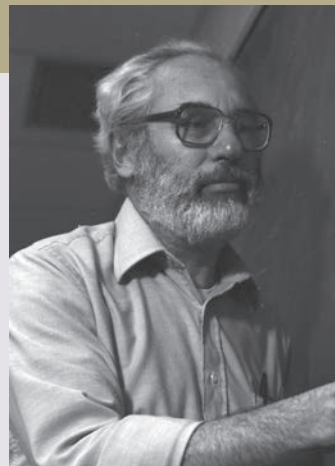
September 21, 1930–February 27, 2016

Elected to the NAS, 1973

Marshall Fixman was a highly original theorist who brought a deep understanding of chemistry and physics, formidable mathematical ability, and profound insight to the fundamental problems in condensed-matter physical chemistry. Equally at home with theoretical methods and computer simulation, he was able to combine both approaches to deepen our understanding of complex physical phenomena.

Early life and education

Marshall was born in St. Louis, Missouri, to Benjamin and Dorothy Fixman. Benjamin was a chemical engineer who had worked for Phillips Petroleum, but after being laid off near the end of the Depression he shifted to retail sales. As a 10-year-old, Marshall became interested in chemistry through a traditional chemistry set and did experiments in the basement of his parents' home that was adjacent to the women's clothing store his father ran. A few years later, when the family moved to University City, Missouri, his parents installed a gas line for his Bunsen burner. By the time he was about 12, Marshall was determined to be a chemist.



Marshall Fixman

By Jeffrey Kovac

Fixman attended University City High School, where he was an excellent student and a member of the chess, track, and cross-country teams. He placed third in the Missouri State Cross-Country Meet in November 1946, which his team won. After high school he attended nearby Washington University in St. Louis, where he was elected to Phi Beta Kappa and graduated in three years with a degree in chemistry. Fixman then went east to pursue graduate work in physical chemistry at the Massachusetts Institute of Technology (MIT), where his research adviser was Walter H. Stockmayer.



Marshall Fixman and Walter H. Stockmayer at Stockmayer's home in Vermont in 1972.

Fixman told the story of his first meeting with Stockmayer after arriving at MIT. He had been making the rounds of the physical chemistry division's research groups in order to decide which team to join, and was standing outside a Stockmayer lab, talking with one of the professor's graduate students. Far in the distance a group of students was moving as one along the busy corridor, surrounding a taller figure who seemed to be their leader. "Who is that," Fixman asked with some contempt, "the student body president?" In fact, it was Stockmayer, who looked much younger than his age.

Fixman joined Stockmayer's research group and the two became lifelong collaborators and friends. They took their first hike in the White Mountains

together in September 1951, followed by many more in New Hampshire, Colorado, and Switzerland. In recognition of Stockmayer's mentorship and the importance of the mountains, Fixman included the following note in his thesis: "Contemplation of the WMNF [White Mountain National Forest] and WHS encouraged the author when nothing else could."

The experimental part of Fixman's thesis involved preparing and fractionating a styrene-methyl methacrylate copolymer, building a differential refractometer, and making numerous light-scattering measurements. He also produced several theoretical results, the most important being the first systematic application of the Mayer cluster-expansion technique to the problem of excluded volume in a flexible polymer chain. As a graduate student, Fixman quickly demonstrated his interest in fundamental problems in physical chemistry. For example, in



Marshall Fixman, Walter H. Stockmayer, and an unidentified person in the White Mountains in 1953.

the “journal meeting” of first-year students, he presented a seminar on David Bohm’s controversial hidden-variable approach to quantum mechanics, which had just appeared in the literature. Not content just to perform light-scattering measurements, he studied Einstein’s fundamental papers on that subject, an effort that would pay off in the future.

Postdoctoral year at Yale and military service

After earning his Ph.D., Fixman went to Yale in 1954 on a Frank B. Jewett Fellowship to work with John G. Kirkwood, one of the preeminent practitioners of statistical mechanics. Future Nobel Laureate Lars Onsager was also a member of the Yale chemistry faculty. Fixman became friends with two other young theorists, Robert W. Zwanzig, then a postdoc with Kirkwood; and Robert Mazo, a Kirkwood graduate student.

Fixman’s primary project was to develop a completely molecular theory of Rayleigh light-scattering by a simple fluid. At the time it was believed by many, including Kirkwood, that the macroscopic fluctuation theory of Einstein was incorrect by a factor that resulted from an internal field, but Fixman’s rigorous analysis showed that Einstein’s result was indeed correct. In this research, Fixman demonstrated two attributes that characterized his entire career: a deep understanding of fundamental physics and chemistry (in this case, electromagnetism and statistical mechanics) and formidable skill in mathematics.

After his year at Yale, Fixman was drafted, and he spent two years as an enlisted man in the U.S. Army. After basic training he was sent to the Rocky Mountain Arsenal, just outside Denver, where he was a member of the Scientific and Professional Personnel component of the Chemical Corps. Fixman’s assignment involved chemical control in the production of chemical warfare agents, which were so corrosive that the production facility was often shut down. He used some of this time off to learn how to ski and climb mountains, both of which became lifelong avocations. But he also used his time away from the lab doing independent research and writing articles, primarily on the theory of liquids.

Harvard University, the Mellon Institute, and the University of Oregon

After his discharge from the army, Fixman was appointed instructor at Harvard University, where he supervised the research of several outstanding graduate students, including John C. Light, Kenneth B. Eisenthal, and Frank C. Andrews. Fixman also pursued his own research on fluctuation theory and transport coefficients in simple liquids, inspired by his year in the Kirkwood group. Fixman’s research at Harvard

exhibited another attribute of his career: most of his best work was done alone. As a result, a large fraction of his bibliography consists of single-author papers.

After Harvard, Fixman spent two productive years (1959–1961) in Pittsburgh at the Mellon Institute of Industrial Research, under the stimulating scientific leadership of future Nobel laureate Paul J. Flory. The Institute, which had been founded in 1913 by Andrew W. Mellon and Richard B. Mellon as a nonprofit independent research center, merged in 1967 with the nearby Carnegie Institute of Technology to form the Carnegie Mellon University.

At the Mellon Institute, Fixman returned to polymer theory, writing several papers on polymer conformations, chain dimensions, and the thermodynamics of polymer solutions. In the latter area, he developed a general theory for the entire range of concentrations—from dilute solutions to undiluted polymer—and he performed the first calculation of the distribution function for the radius of gyration of a Gaussian chain. He then moved into a new area—critical phenomena—and laid the foundation for what was later known as mode-coupling theory. Because density fluctuations become long-ranged, extending as much as thousands of angstroms near the critical point, it was important to learn how much these long-range fluctuations affected the transport properties such as viscosity. Fixman considered this problem in several papers, offering insights that were crucial to the development of the modern theory of transport in the critical region. He also contributed several extensions of the classical theory of equilibrium critical phenomena.

In 1961, Fixman moved to the University of Oregon, where he had been appointed professor of chemistry and director of the newly established Institute of Theoretical Science. During the Great Depression, as an economy move the State of Oregon had moved all upper-division and graduate-science education to Oregon State University. But after World War II, with rising enrollments and increased state revenues, the University of Oregon's administration received permission to rebuild its science departments. In this fertile environment, Terrell L. Hill, a distinguished theorist who was a member of the Department of Chemistry, championed the formation of interdisciplinary institutes. The first, established in the late 1950s, was the Institute of Molecular Biology, which linked chemistry and biology; the second, formed in 1961, was the Institute of Theoretical Science.

On the face of it, Fixman's appointment was surprising. He was only 31 years old, and his single previous academic appointment had been as an instructor at Harvard. But the

department's confidence in him was justified when in 1964 Fixman won the American Chemical Society's Award in Pure Chemistry—a prize bestowed on an outstanding chemist with fewer than 10 years of experience since receiving the terminal degree. Fixman was soon joined at the Institute by his friend from Yale, Robert Mazo.

At Oregon, Fixman continued his work on critical phenomena and polymer conformations and thermodynamics; he also expanded his interests to include nonequilibrium polymer problems. A major theme for the remainder of his career was polymer dynamics. As was typical of Fixman's work, he began by formulating a mathematically elegant general theory of polymer dynamics that could then be applied, with approximations, to specific problems. He introduced two perturbation theories to incorporate the effects of excluded volume, fluctuating hydrodynamic interactions, and high strain rates—effects that could not be explained in the context of the standard Rouse-Zimm theory.

The Yale years

In 1965, Fixman moved to Yale University, where he had been appointed professor of chemistry and would eventually become the Eugene Higgins Professor of Chemistry. There he supervised numerous graduate students and postdoctoral research associates. Seven graduate students—Kenneth L. Rider, John Bendler, Gerald Wilemski, Robert Cook, Branka M. Ladanyi, Jeffrey Kovac, and Jeffrey Skolnick—half his career total, received their Ph.D.s under his direction during his 14 years at Yale. He also worked with several excellent research associates, including Bruce Eichinger, Juan Friere, and

Glenn T. Evans. Most of Fixman's research involved the conformation and dynamics of polymers, but he also made notable contributions to the theory of highly anharmonic crystals, liquid crystals, the helix-coil transition, and polyelectrolytes. In 1973, he was elected to the National Academy of Sciences.

Early in his time at Yale, Fixman developed a sophisticated extension of his general theory of polymer dynamics. He first approached the original matrix formulation of the equation of motion using a Hermite function basis set. This



Yale Graduate Students – Robert Cook, Jeffrey Kovac, and Branka Ladanyi.

suggested the introduction of an operator representation in which the operators obeyed Boson commutation relations, which facilitated the application of the theory to include the excluded volume effect. He then incorporated the constraints of constant bond length and bond angle into the theory of polymer dynamics.

The classic Rouse-Zimm theory modeled the polymer chain as a series of point centers with spring-like connectors. This model gave the correct conformational statistics in a theta solvent and an explanation of the dynamic properties of dilute solutions at low frequencies. The Rouse-Zimm theory predicted that the dynamic viscosity vanishes at high frequency, but this contradicted experimental results that showed a finite value for the viscosity. This finite viscosity resulted from the chain's short-range stiffness due to bond length and bond angle constraints. In collaboration with graduate student Jeffrey Kovac and research associate Glenn T. Evans, Fixman developed a theory that incorporated these constraints.

Fixman worked with his Yale graduate students on several other projects. For example, he and Gerald Wilemski developed a theory of diffusion-controlled reactions and applied it to the problem of interchain reactions in polymers. And Fixman and Jeffrey Skolnick studied polyelectrolytes in which charge interactions strongly affect the chain conformation. Near the end of his time at Yale, Fixman recognized that the increasing power of digital computers made it possible to do realistic simulations of polymer systems, and he began using them to help develop both the fundamental theory and the algorithms for solving important problems in polymer dynamics. This area became a major pursuit during the remainder of his career.

Colorado State University

In 1979, Fixman moved to Colorado State University as a professor of chemistry and physics. In 1986, he was named University Distinguished Professor, CSU's highest faculty position. Along with continuing his research, done mostly alone but also in collaboration with several postdocs and his last graduate student, Komala Krishnaswamy, Fixman served as associate editor of the *Journal of Chemical Physics* from 1994 to 2006.

He formally retired from Colorado State in 2000, but continued to do research to the end of his life. For example, Fixman developed computer-simulation methods to study the dynamics of concentrated solutions and undiluted polymers, and his theoretical and simulation results emphasized a more active role for the environment of a test molecule. One of his most significant results showed the inadequacy of the concept of a fixed cage

hemming in a primitive reference chain, as postulated by the simple reptation model. Polyelectrolytes continued to interest him, and he developed both theoretical and simulation methods to study their equilibrium and dynamic properties. This led to research on the electrokinetics of macroions and electrophoresis. His final article, left unfinished at his death, was on electrokinetics.

Family and personal life

During his last year at Harvard, one of Fixman's graduate students met an attractive young woman, Marian Beatman, at a cocktail party. Beatman, a graduate of Wellesley College and the Harvard Graduate School of Education, was an editor at Allyn & Bacon, Inc., a textbook publisher in Boston. After talking with her, the student became convinced that she was just the right person for Fixman. He was correct, and Fixman and Beatman were married in July 1959. They had three children: Laura, (1960–2015), Susan (b. 1962), and Andrew (b. 1964). Marian Beatman died in 1969.



Marshall Fixman and Branka Ladanyi in 2010.

In 1974, Fixman married Branka M. Ladanyi, who had been one of his Yale graduate students. A major reason why he moved from Yale to Colorado State was that the

chemistry department at CSU had offered Ladanyi a position as assistant professor. She enjoyed a very successful research career there, and they were happily married for 42 years. Ladanyi died on January 30, 2016, and Fixman died a month later, on February 27, 2016.

Fixman had a great love of the outdoors, particularly skiing and hiking. He especially enjoyed the mountains of New Hampshire and Colorado, but also took the opportunity to hike in new places whenever he could. He was an outstanding photographer who developed his own photos in his home darkroom. On hiking trips he often carried no fewer than three cameras. At his death, he left many T-byte drives filled with high-resolution photos scanned from film and slides, as well as more recent digital images.



Marshall Fixman on the Appalachian Trail at the Maine-New Hampshire border.

Honors and awards

In addition to the ACS Award in Pure Chemistry, Fixman won the American Physical Society's High Polymer Physics Prize in 1980 and the American Chemical Society's Award in Polymer Chemistry in 1991. Early in his career he was an Alfred P. Sloan Fellow and in 1988 won the Senior U.S. Scientist Award from the Alexander von Humboldt Foundation. Fixman was a fellow of both the American Academy of Arts and Sciences and the American Physical Society.

Reflections

His powers of concentration were astounding. As a graduate student, if I arrived at an appointment to discuss my own research and he had been working on something, it would take him several minutes to shift focus. He was almost always able to get to the essence of things. After listening to a lecture at a department seminar or a scientific meeting he would ask a deep probing question concerning the basis of the research. His questions were never asked to show up the speaker; he just wanted to understand. Fixman avoided popular areas of research, instead following his own interests and instincts. And once he became interested in something, he almost always was able to make a fundamental advance. The scope of his research over 60 years was astounding. Although there were but two major themes—polymer theory, including polyelectrolytes and DNA; and critical phenomena—the range of problems within those areas was wide. Fixman’s approach to a problem was usually quite original, and he was often able to take what he learned in one area and apply it to something in another area.

As noted, Fixman did much of his best work alone. He was happy to have collaborators such as graduate students and research associates, and he interacted well with them, but he always had his own research. Fixman suggested interesting problems for his collaborators to work on and then gave them independence; he was available to help, but never put pressure on a coworker to finish a project. When you went to Fixman for assistance, he would listen patiently, puff on his ever-present corn cob pipe, and provide excellent suggestions, although I remember that it often took me several days to really understand them. His former students and postdocs remember him as a fine mentor who had a profound influence on their careers.

Fixman was a very private person. As a graduate student he often went off into the mountains alone, where he studied the writings of New England writers, particularly Henry David Thoreau, whom he regarded as a professional theorist of life. In the early 1970s he had a semester’s leave from Yale and spent much of it hiking the Appalachian Trail by himself. He believed that theoretical thinking tends to mature when conscious of reality but away from it. He once commented that theorists were those who heard voices. I suspect he did not have anything mystical in mind, but rather that theorists were able to go deeply into their own heads and, in the words of Einstein, discover “the secrets of the Old One.” Like Thoreau, Fixman loved nature and savored his time in the mountains observing. Photography was one of the ways he observed, and many of his photos were startlingly good.



Photograph by Marshall Fixman.

Fixman always thought before he spoke. He wasn't very talkative but when he did speak, his words had meaning. He had a serious demeanor but also had a good sense of humor and enjoyed the company of others. He was engaged and interested in the world around him, both the natural world and human events. Through his teaching, personal interactions, and writing, he was a mentor and inspiration to several generations of theorists.

SOURCES

A biographical article on Marshall Fixman by Elliot R. Bernstein and Walter H. Stockmayer was published in 1992 in the *Journal of Physical Chemistry* 96:3911–3912. Fixman's son Andy provided me with a variety of materials, including an article from the Eugene Register-Guard (September 13, 1963) and notes that Fixman had written for a biographical memoir of Walter H. Stockmayer. Several of Fixman's former students, research associates, and colleagues sent recollections. I am grateful to John Bandler, Robert Cook, Glenn Evans, Komala Krishnaswamy, Nancy Levinger, Robert Mazo, Grzegorz Szamel, Dub Shults, and Harry Workman for sharing their memories with me.

SELECTED BIBLIOGRAPHY

- 1953 With B. H. Zimm and W. H. Stockmayer. Excluded volume in polymer chains. *J. Chem. Phys.* 21:1716–1723.
- 1955 With W. H. Stockmayer, L. D. Moore, Jr., and B. N. Epstein. Copolymers in dilute solution. *J. Polyp. Sci.* 16:517–530.
- Molecular theory of light scattering. *J. Chem. Phys.* 23:2074–2079.
- 1960 Density correlations, critical opalescence, and the free energy of non-uniform fluids. *J. Chem. Phys.* 33:1357–1362.
- 1961 General theory of polymer solutions. *J. Chem. Phys.* 35:889–894.
- 1962 Radius of gyration of polymer chains. *J. Chem. Phys.* 36:306–310.
- Viscosity of critical mixtures. *J. Chem. Phys.* 36:310–318.
- 1963 The critical region. In *Advances in Chemical Physics*, Volume 6. Edited by I. Prigogine. Hoboken, NJ: John Wiley & Sons.
- 1965 Dynamics of polymer chains. *J. Chem. Phys.* 42:3831–3837.
- 1966 Polymer dynamics: Boson representation and excluded-volume forces. *J. Chem. Phys.* 45:785–792.
- 1969 Highly anharmonic crystal. *J. Chem. Phys.* 51:3270–3279.
- 1973 With G. Wilemski. General theory of diffusion-controlled reactions. *J. Chem. Phys.* 58:4009–4019.
- 1974 With G. Wilemski. Diffusion-controlled intrachain reactions of polymers. I. Theory. *J. Chem. Phys.* 60:866–877.
- With J. Kovac. Dynamics of stiff polymer chains. I. *J. Chem. Phys.* 61:4939–4949.
- 1976 With G. T. Evans. Dynamics of stiff polymer chains IV. High-frequency viscosity limit. *J. Chem. Phys.* 64:3474–3480.
- 1977 With J. Skolnick. Electrostatic persistence length of a wormlike polyelectrolyte. *Macromolecules* 10:944–948.
- 1978 Simulation of polymer dynamics. I. General theory. *J. Chem. Phys.* 69:1527–1537.

- 1981 Inclusion of hydrodynamic interactions in polymer dynamical simulations. *Macromolecules* 14:1710–1717.
- 1983 Variational bounds for polymer transport coefficients. *J. Chem. Phys.* 78:1588–1593.
- 1985 Dynamics of semidilute polymer rods: An alternative to cages. *Phys. Rev. Lett.* 55:2429–2432.
- 1988 Chain entanglements. I. Theory. *J. Chem. Phys.* 89:3892–3911.
- 1990 Polyelectrolyte bead model. I. Equilibrium. *J. Chem. Phys.* 89:3892–3911.
Models of polymer and solvent dynamics *J. Chem. Phys.* 92:6858–6866.
- 2004 Scattering from polydisperse melts. *Macromolecules* 37:8441–8456.
- 2006 A macroion electrokinetics algorithm. *J Chem. Phys.* 124:1–19.

Published since 1877, *Biographical Memoirs* are brief biographies of deceased National Academy of Sciences members, written by those who knew them or their work. These biographies provide personal and scholarly views of America's most distinguished researchers and a biographical history of U.S. science. *Biographical Memoirs* are freely available online at www.nasonline.org/memoirs.