



Walter Kohn

1923–2016

BIOGRAPHICAL

Memiors

*A Biographical Memoir by
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and J. S. Langer*

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NATIONAL ACADEMY OF SCIENCES

WALTER KOHN

March 9, 1923–April 19, 2016

Elected to the NAS, 1969

Walter Kohn, a giant of theoretical physics, died at his home in Santa Barbara, California on April 19, 2016, at the age of 93.

Walter's life epitomized both the hardships and the wondrous achievements of physicists in the 20th Century. He escaped from Nazi occupied Austria on one of the last children's rescue trains (the "Kindertransport") and during World War II spent eighteen months confined in internment camps in England and Canada. He learned only after the war that both of his parents had been murdered in Auschwitz. After earning physics degrees at the University of Toronto and at Harvard, he rapidly emerged as a leader in bringing quantum theory to bear on problems in the electron theory of solids. Walter's devotion to basic scientific principles led in the 1960's to the density-functional theory of electrons in solids and in chemical molecules. Thirty years later, once the vast importance of this theory had become clear, he was awarded a Nobel Prize in Chemistry for this discovery. In his later years Walter turned much of his attention to institution building and public affairs. He was the founding director of the Institute for Theoretical Physics at the University of California, Santa Barbara. He was deeply committed to the control of nuclear weapons, the development of renewable clean energy, and the free exchange of knowledge among scientists throughout the world.



A handwritten signature in black ink that reads "W. Kohn". The signature is written in a cursive style.

By P. C. Hohenberg
and J. S. Langer

This biographical memoir is largely a personal account by its authors, Hohenberg and Langer. Walter Kohn touched our lives in deep and meaningful ways that we shall try to describe throughout this memoir. To emphasize this personal flavor we include several first-person accounts and quote Kohn's own words at times (mostly from his Nobel autobiography). [1] For an in-depth discussion of the development of Walter's scientific ideas we strongly recommend the perceptive paper by A. Zangwill. [2]

What we remember most clearly is Walter's joy in scientific discovery and his strong sense of personal integrity. We hope to make these characteristics clear in what follows.

Walter Kohn was born in 1923 into a well educated, middle class Jewish family in Vienna. His father Salomon owned a publishing company that specialized in high-quality art postcards, mostly based on contemporary paintings. The business flourished in the first two decades of the century but fell on hard times after World War I. His mother Gittel was fluent in many languages and strongly encouraged her son to obtain a humanistic education. Accordingly, Walter was enrolled in Vienna's prestigious Akademisches Gymnasium where he excelled at Latin and ancient history but, as he said later, showed "no interest in, nor apparent talent for mathematics." [1]

When Nazi Germany annexed Austria in 1938, Jews were expelled from the Akademisches Gymnasium and all other public schools. Walter was able to enter a Jewish school, the Chajes Gymnasium where, in his words:

I had two extraordinary teachers: In physics, Dr. Emil Nohel, and in mathematics Dr. Victor Sabbath. While outside the school walls arbitrary acts of persecution and brutality took place, on the inside these two inspired teachers conveyed to us their own deep understanding and love of their subjects. I take this occasion to record my profound gratitude for their inspiration to which I owe my initial interest in science. (Alas, they both became victims of Nazi barbarism). [1]

In August of 1939, Walter's parents succeeded in sending him to England on one of the last of the Kindertransport trains that was allowed to pass through Germany. As a refugee, he was taken in by a British family in Sussex (Charles and Eva Hauff) who had welcomed his sister Minna a year earlier. He enrolled in a local school where he studied English and began concentrating in mathematics and science. However, having arrived carrying a German passport, he was interned as an enemy alien in May 1940, along with tens of thousands of foreign residents in England. He was detained in various internment camps, first in England and then, after a dangerous voyage in a troop ship across the Atlantic, in Canada.

The population of the Canadian internment camps at which Walter spent the next year and a half consisted in large part of Jewish refugees who established their own internal organizations. Especially important for Walter was a camp school where he was able to continue studying physics and mathematics. He now took these subjects extremely seriously, going so far as to save the small amount of money that he earned working at the camps to buy textbooks by G. H. Hardy and J. C. Slater. Those books were still on his shelves in 2016. By September 1941, he was part of a group of young internees who were

permitted (under guard) to take McGill University's Senior Matriculation Examination, in which he did extremely well.

Life changed decisively for Walter in the fall of 1941. He and his life-long friend and fellow Viennese refugee Josef (Terry) Eisinger were invited by Hertha and Bruno Mendel to live with them in Toronto, thereby enabling them to be released from the internment camps. The Mendels had chosen Walter and Terry among other teenagers in internment because they had been told that the two boys played recorder duets together in the camp. The music-loving Mendels were German Jewish refugees who had emigrated to Canada in 1937. Along with their three children, they had brought with them Hertha's mother Toni who had been a friend of Albert Einstein since the early 1920s. In Berlin she had lived in a magnificent home named Villa Wannsee where her son-in-law Bruno had built a private laboratory for his cancer research. Einstein had visited that laboratory and had advised Bruno on technical matters. In Canada Bruno had found a medical-science position at the University of Toronto. There he became a friend of the Polish general relativist Leopold Infeld who had worked with Einstein at Princeton.

In the early 1940's Walter was planning to study engineering rather than physics in order to be able to support his parents after the war. However, the Mendels introduced him to Infeld who, after talking with him in a kind of drawing room oral exam, concluded that Walter's real love was physics and advised him to major in the rigorous Math-Physics program at the University of Toronto. He argued that this program would enable Walter to earn a decent living at least as well as an engineering program.

By the summer of 1945 Walter had completed the course requirements for his Toronto undergraduate degree and was finishing a year in the Canadian army. He had taken courses with a distinguished and stimulating group of mathematics and physics professors and he already had begun to do research on his own. In fact, his first substantial publication (on the theory of spinning tops) [3] was finished and submitted in November, 1944, at a time when he was engaged in basic military training at an army base in Ontario. At the end of the war he returned to Toronto for one more year to finish the requirements for a Master's degree. Then, in the fall of 1946, again with advice from Infeld, he accepted a fellowship for graduate studies at Harvard.

Walter arrived in Cambridge just as large numbers of young scientists and engineers were converging on Harvard and M.I.T. to switch from defense-related work to academic research. Among the new colleagues he mentioned in his Nobel autobiography were Philip Anderson, John Blatt, Nicolas Bloembergen, Kenneth Case, Frederick de Hoffman, Roy

Glauber, Marvin Goldberger, Thomas Kuhn, Rolf Landauer, Joaquin Luttinger, Ben Mottelson, George Pake, and Charles Slichter—all of whom went on to highly distinguished scientific careers. As advised by Infeld, he applied to Julian Schwinger and was accepted as one of ten new Ph.D. students. Apparently none of Schwinger's students at that time had close relations with their supervisor, who was deeply engrossed in the fundamental problems of quantum field theory. Walter was no different from the others, and recalled being unhappy about how few meetings he had with his supervisor. Nevertheless, when Schwinger died in 1994, Walter wrote the following tribute to him:

It was during these meetings, sometimes more than 2 hours long, that I learned the most from him...to dig for the essential; to pay attention to the experimental facts; to try to say something precise and operationally meaningful, even if one cannot calculate everything a priori; not to be satisfied until one has embedded his ideas in a coherent, logical, and esthetically satisfying structure... [4]

These words say at least as much about Walter Kohn's scientific philosophy as they do about Julian Schwinger's.

In 1948, just two years after arriving at Harvard, Walter completed a PhD thesis on the quantum-mechanical description of "Collisions of Light Nuclei," and claimed to have been surprised when Schwinger asked him to stay on as a research assistant with some teaching responsibilities. He accepted and, with the security of a real job, married Lois Adams whom he had met in Toronto. The two soon produced the first of their three daughters. Walter did continue working with Schwinger, but these were the years in which Walter's interests shifted into solid state physics. The transition happened with encouragement from John Van Vleck, then chair of the Harvard Physics Department, who had been discussing solid state problems with Walter. Van Vleck invited Walter to teach a graduate solid-state course in the fall of 1949, which seems to have been an intensive learning experience. His students included Bloembergen, Slichter, and Pake. As a measure of how rapidly his life was moving in those years, he published a paper [5] with Bloembergen in 1950 on a theory of the newly discovered Knight shift in nuclear magnetic resonance.

By the spring of 1950 Walter was looking for a more permanent job. He was offered a faculty position in the Physics Department at Carnegie Institute of Technology (now Carnegie Mellon University) in Pittsburgh, starting in the fall of 1950. However, he then learned that he had won a National Research Council Fellowship that would support

him for a year in Europe. So he delayed moving to Pittsburgh and took his family to Niels Bohr's Institute for Theoretical Physics in Copenhagen in January 1951. Walter was expanding his scientific contacts as international physics was reviving after the War. Bohr held a Conference on Problems in Quantum Physics in July 1951, attended by many of the world's leading theorists. That summer Walter gave a course on solid state physics at the first of the Les Houches summer schools. He also briefly visited Rudolf Peierls' very active Department of Mathematical Physics in Birmingham, England. With Bohr's endorsement, he was awarded an Oersted Foundation fellowship that allowed him to remain in Copenhagen through the summer of 1952. This was the year in which he collaborated with the Swiss theorist Res Jost in developing quantum theories of particle scattering. Kohn and Jost remained close friends for many years.

Back in the U.S. at Carnegie Tech in the fall of 1952, Walter played a central role in building a strong research program in solid state physics. In collaboration with the Canadian post-doc Norman Rostoker he developed what became known as the Kohn-Korringa-Rostoker method for computing electronic band structures in metals. [6] Later in that decade he developed his theory of the "Kohn anomalies" in which he showed how the Fermi surface that describes the electronic states in metals can be seen as a singular feature of the vibrational spectra of these solids. [7]

In 1953 Walter began a summer consulting relationship with Bell Laboratories in New Jersey. According to him:

Bell Labs at that time was without question the world's outstanding center for research in solid state physics and, for the first time, gave me a perspective over this fascinating, rich field. Bardeen, Brattain, and Shockley, after their invention of the transistor, were the great heroes. Other world class theorists were C. Herring, G. Wannier and my brilliant friend from Harvard, P. W. Anderson. With a few interruptions I was to return to Bell Labs every year until 1966. I owe this institution my growing up from amateur to professional. [1]

It was also at Bell Labs in the summer of 1954 that Walter began his close collaboration with Joaquin ("Quin") Luttinger that produced, among other important advances, an effective mass theory of electrons and impurities in semiconductors [8] and a derivation of the Boltzman transport equation for quantum mechanical particles. [9]

Walter was immersed in educational as well as research activities at Carnegie Tech. It was in this capacity that he first crossed paths with one of the present authors (JSL, adapted from [10]):

In the fall of 1954 I was in my last year as an undergraduate physics major and Walter was a junior member of the faculty. I no longer remember whether Walter volunteered or was drafted for the responsibility, but somehow he became my private instructor for a year-long supervised reading course in quantum mechanics. We went through the first edition of Schiff's classic text, doing most of the problems and often talking about the ways in which those ideas were being used in current research.

I recall many such discussions, many times when I didn't think I was catching on as quickly as I thought I should, and many other times when I thought I was being given keys to the secrets of the universe. I especially remember the time when Walter arrived at his office with an intense gleam of triumph in his eye and announced that he had just done something 'fiendishly clever.' The achievement was possibly his calculation of the energy levels of impurities in semiconductors, a calculation that I could have followed at that time, and possibly did. His enthusiasm made a lasting impression. I never shall forget his joy in the discovery and my hope that I might some day have that kind of experience.

When, during that year, I learned that I had won a Marshall Scholarship to be used at any British university, it was Walter who wisely steered me toward Peierls in Birmingham.

Walter remained at Carnegie Tech until 1960 when he moved to the newly created campus of the University of California at San Diego. The main campus of UCSD had yet to be built atop the hills overlooking the ocean near La Jolla; and the new physics department was temporarily located near the beach in a building that belonged to the Scripps Institute of Oceanography. The building was undistinguished, but the location was spectacular, especially on days when the surf was high. Walter immediately began to build his own research group there. However, in the spring of 1961, the founding department chair Keith Brueckner accepted a position at the Institute for Defense Analysis in Washington D.C., and Walter was less than thrilled to discover that he would have to take over the chairmanship. In addition to supervising a graduate curriculum and

maintaining his research program, he would be responsible for recruiting about a dozen new faculty members. Thus Walter became an institution builder.

Starting in the late 1950's, solid-state theory had undergone a major transition with the realization that the problems of interacting electrons in solids could be tackled using the methods of quantum field theory. Those methods had been successful in solving problems in quantum electrodynamics and were making useful progress in elementary-particle physics. They were perturbative methods, which means that they were expansions in powers of the strength of the interactions between the particles. A great deal of effort was spent in trying to extend these methods to many-body problems in nuclear and solid-state physics where the interactions are strong and perturbative approximations are problematic.

Walter Kohn was very much at the center of these developments, starting with his Ph.D. thesis on nuclear scattering theory. However, beginning with his earliest mathematical experiences in Canada, he had also been interested in non-perturbative techniques. He was especially interested in variational methods with which, for example, one might try to minimize an exact expression for the energy of a many-particle system in order to predict its ground-state properties. In 1961 he was awarded the American Physical Society's Oliver Buckley Solid State Physics Prize. Thus, by the early 1960's, he was a recognized leader in solid-state physics with an unusually broad range of theoretical insights.

Walter's term as department chair at UCSD lasted through the summer of 1963. Then, with support from the Guggenheim Foundation, he spent the fall semester of that year at the École Normale Supérieure in Paris, occupying part of the spacious office of his colleague Philippe Nozières. There, in collaboration with one of the present authors (PCH), he initiated the work that was to become his most famous contribution to science and was to lead to his Nobel Prize (in Chemistry!) in 1998 – namely, the development of what is known as “density functional theory.”

In their first (1964) paper, [11] Hohenberg and Kohn presented an exact, variational reformulation of many-body quantum theory in which the usual set of multi-variable wave functions was replaced by a single position-dependent density of electrons. This was a remarkable result both in its rigor and its generality. The systems to which it could be applied consisted of arbitrarily large numbers of electrons in the presence of arbitrary arrangements of atomic nuclei. Examples that seemed most interesting at the time were crystalline solids containing random arrays of impurities; but this Hohenberg-Kohn theorem applied equally well to chemical molecules of arbitrary complexity.

Here is Hohenberg's account of his historic early interaction with Walter Kohn (PCH adapted from [10]):

I first met Walter Kohn in 1963 when I was a fresh Ph.D. spending a post-doc year in Paris at the École Normale Supérieure in the group of Philippe Nozières. As it happened, Walter was also spending time at the École Normale and conditions being what they were I was privileged to share an office with him for an extended period. If I remember correctly, the relatively large space was Philippe's office and even if it wasn't I remember it to have been a general meeting place and thoroughfare, a little bit like trying to think deep thoughts in the middle of Times Square.

In any event, soon after I met Walter he did me the honor of inviting me to join him in a new research project he was undertaking, the examination of theoretical methods for treating an inhomogeneous electron gas. To say that this project turned out to be successful is a singular understatement, since the paper we produced in the Spring of 1964 [11] was one of two works cited by the Nobel Committee in awarding the 1998 Chemistry Prize to Walter. At the time I remember that it felt like being led through an enchanted, and at times haunted, forest by a trusted guide.

Returning to San Diego in January 1964, Walter and his new postdoctoral associate Lu Sham recast the Hohenberg-Kohn theory in terms of an exact set of generalized quantum many-body (Hartree-Fock) equations expressed once again entirely in terms of the electron density. [12] The Hohenberg-Kohn and Kohn-Sham papers [11,12] were listed by Redner [13] in 2005 as the most highly cited publications in the 100-plus year history of the *Physical Review*. The reason for the enormous impact of this work is that it produces useful approximate solutions of the many-body quantum mechanical equations with no more difficulty than the more conventional Hartree-Fock method, but with significantly better accuracy. As a result, the method has been employed in a huge number of calculations of the electronic structure of solids and, since the 1980s, has been used by chemists to predict the properties of complex atoms and molecules.

Walter kept UCSD as his base of operations through the 1960's and 1970's. He travelled widely, including regularly to Bell Labs, and he continued to broaden his interests. For example, he and Luttinger published an interesting paper on superconductivity in 1965. [14] At the same time, he continued his development of density functional theory and increasingly was trying to convince the chemists to pay attention to this technique. One

of the first to do so was Robert Parr, who had met Walter when they were both briefly at Carnegie Tech in the early 1950's. According to Walter, Parr was "the first major theoretical chemist to believe in the potential promise of density functional theory for chemistry." [1] However, it was not until the 1980's and 1990's, with the advent of fast powerful computers, that density functional theory became the predictive method of choice for research in materials physics and chemistry.

Walter was remarried in 1978, to Mara Vishniac, the daughter of the photographer Roman Vishniac and, like Walter, a Jewish refugee from Nazi oppression.

In 1979, Walter was recruited by the University of California at Santa Barbara (UCSB) to be the founding director of the Institute for Theoretical Physics (ITP) (now called the Kavli Institute for Theoretical Physics). In the opinion of the present authors, Walter's leadership of the ITP was as important for the progress of modern physics as were his prize winning scientific accomplishments.

The idea for such an institute started with Boris Kayser at the National Science Foundation, who thought that theoretical physics needed some analog of a national laboratory. He solicited proposals, brought finalists to Washington to make presentations, and ultimately awarded the grant to UCSB. The authors of the UCSB proposal were James Hartle, Raymond Sawyer, Douglas Scalapino, and Robert Sugar. Their plan was that the ITP would host about four different resident research programs per year, each focusing on a specific set of emerging research problems, and each involving ten or twenty visiting participants at any time. To provide expertise and continuity for these activities, the ITP would have a Director and a small group of permanent members, a group of postdoctoral associates in residence for two years or more, and a broadly representative external advisory board. The incoming UCSB Chancellor, Robert Huttenback, played a key role by promising the resources needed to make this plan feasible.

Walter led the ITP to a strong start. With Sugar as the first Deputy Director, and with a small but remarkably capable administrative staff led by Bonnie Sivers, the ITP quickly established an effective mode of operation for itself. Its activities had a multidisciplinary flavor from the very beginning. There were research programs in neural networks and nonequilibrium dynamics as well as activities in particle and nuclear physics, astrophysics and condensed matter (the new name for solid-state) physics. Walter personally created a unique environment for wide-ranging and innovative research, and he also set the tone for warm, thoughtful guidance of promising young scientists. Under Walter's leadership,

the ITP quickly became a destination of choice for scientists throughout the world. It has remained so to this day.

Walter Kohn played a positive role in the lives of a great many people, of whom only a small fraction are mentioned in this memoir – mostly those with whom he interacted scientifically. (For more complete accounts of and by his colleagues, see the collection of personal notes published by Matthias Scheffler and Peter Weinberger on the occasion of Walter's 80th birthday. [10]) But Walter was also a warm human being with deep concerns about issues of political, national and international significance. To communicate the depth of his concerns, we quote again from his Nobel autobiography:

I want to mention that I have a strong Jewish identity and – over the years – have been involved in several Jewish projects such as the establishment of a strong program of Judaic Studies at the University of California in San Diego.

My father, who had lost a brother fighting on the Austrian side in World War I, was a committed pacifist. However, while the Nazi barbarians and their collaborators threatened the entire world, I could not accept his philosophy and, after several attempts, was finally accepted into the Canadian Infantry Corps during the last year of World War II. Many decades later I became active in attempts to bring an end to the US-Soviet nuclear arms race and became a leader of unsuccessful faculty initiatives to terminate the role of the University of California as manager of the nuclear weapons laboratories at Los Alamos and Livermore. [1]

Walter also was active in efforts within the scientific community to defend the human rights of scientists throughout the world. He was deeply committed to environmental issues. In 2005, he joined fellow UCSB Nobelist Alan Heeger to produce the film *The Power of the Sun* [15], advocating greater attention to the promise of sustainable energy sources.

Walter Kohn will long be remembered by colleagues and friends, near and far.

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We are especially grateful to Mara Kohn, both for playing such a central role in the last decades of Walter's life and for her thoughtful guidance to us in writing this memoir.

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