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# ELLIOTT WATERS MONTROLL

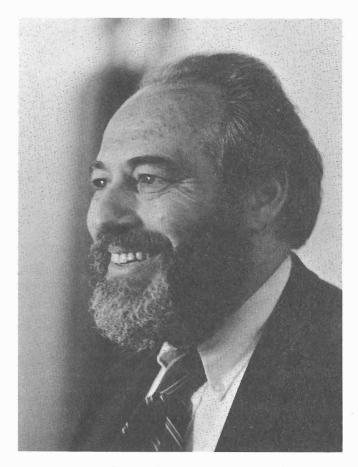
## 1916—1983

A Biographical Memoir by GEORGE H. WEISS

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Biographical Memoir

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## ELLIOTT WATERS MONTROLL

### May 4, 1916–December 3, 1983

BY GEORGE H. WEISS

LLIOTT W. MONTROLL was born on May 4, 1916, to Adolph L B. and Esther I. Montroll in Pittsburgh, Pennsylvania. His father, an immigrant from Poland, and his Americanborn mother encouraged him from an early age to pursue his interests in chemistry, which he did in high school as well as in his undergraduate studies at the University of Pittsburgh. However, after receiving his bachelor's degree in chemistry, Elliot switched fields as a graduate student, receiving his Ph.D. in mathematics at the age of twentythree. A forerunner of his later interests, Elliot's thesis was on application of the theory of integral equations to the evaluation of integrals that appear in the analysis of imperfect gases.<sup>1</sup> The techniques developed in his thesis were based on linear operator theory and Fourier integrals. These tools were to prove the cornerstone to a significant portion of Elliot's future work.

Following the receipt of his doctorate, Elliott spent three years as a postdoctoral fellow working for a year at Columbia with Joseph Mayer, followed by a year as a Sterling fellow at Yale with Lars Onsager, and finally spending a year with John Kirkwood at Cornell. After this period of study, he accepted an instructorship at Princeton in 1942. It was at the last of these that Elliott met his future wife, Shirley Abrams, whom he married in 1943. Their marriage was an unusually warm and happy one, producing ten children over the years. Much of Elliott's fertile imagination was devoted to producing new and novel ways to educate his children.

During the war Elliott worked at the Kellex Corporation in New York City as a chief mathematician analyzing problems arising in the production of the atomic bomb. This work also served as a source of techniques that he later developed and applied in other scientific fields. Following the war Elliott briefly held teaching and research positions at Brooklyn Polytechnic Institute and the University of Pittsburgh. He later became the director of physical science at the Office of Naval Research, after which he returned to the world of research, spending a year as a fellow at the Courant Institute in New York City.

In 1951 the Montrolls returned to the Washington area, and Elliott took a position as a research professor at the Institute for Fluid Dynamics and Applied Mathematics at the University of Maryland. During this time he spent a sabbatical period with Ilya Prigogine at the Free University of Brussels, and he held the position of Lorentz Professor at the University of Leiden in 1961. Following this period at the University of Maryland, Elliott decided that he wanted to get a taste of industrial research, several of his doctoral students having gone into industry, and so he left the University of Maryland to become a vice-president in charge of physics research at IBM, a position he held for three years, during which time he also acted as a consultant for the Institute for Defense Analysis. After having been the director of general sciences at IBM, Elliott took on the position of vice-president of the Institute for Defense Analysis.

In 1966 he accepted an offer of an Einstein professorship at the University of Rochester, which he held until 1981 when he returned to the Institute for Physical Science and Technology at the University of Maryland. Subsequent to his appointment he was named a distinguished professor at the university in 1982. This position was held until his death.

The time that Elliott spent at universities produced a large number of doctoral students. His research groups, always extensive, provided a lively intellectual atmosphere and were filled with many junior and senior postdoctoral investigators, all working on a variety of topics as befitted Elliott's wide-ranging research interests. His catholic tastes and interest in topics outside of science proper produced many unusual contributions to disciplines outside of mathematical physics and led to his teaching such courses as "Quantitative Aspects of Social Phenomena" and "The Physical Basis of Modern Technology" at the University of Rochester.

Elliott's scientific style was extremely elegant, producing insight into often difficult physical problems usually by means of very simple calculations. One of his earliest pieces of work resulted in the publication, together with Joseph Mayer, of a technique for the summation of the contribution of the class of ring diagrams in the diagrammatic analysis of the theory of imperfect gases.<sup>2</sup> This seminal contribution proved to be the forerunner of a powerful technique subsequently adapted by many investigators to analyze a variety of problems in both equilibrium and irreversible statistical mechanics. A second, slightly less successful investigation was carried out while Elliot was a postdoc with Lars Onsager into the solution of the Ising model. Elliott developed a technique for solving the partition function of the Ising model but was only able to solve the one-dimensional case exactly and find high- and low-temperature expansions for the partition function in two dimensions. Onsager, of course, provided an exact solution in two dimensions which, for the first time, showed that the mathematical formalism indeed predicted a phase transition for this model.

Although it was not Elliott who solved the Ising model, his work on it led to other significant contributions. For many years a review article by Newell and Montroll on the Ising model was the most readable and most widely cited introduction to the subject.<sup>3</sup> A second bonus of Elliott's work on the Ising model consisted of some work first published in the Journal of Chemical Physics in the context of the Ising model.<sup>4</sup> After the mathematical ideas had been distilled from this work Elliot published an elegant extension of it in the Annals of Mathematical Statistics.<sup>5</sup> This later paper contained a general and easily applicable formalism for calculating the probability distribution of functions defined on a Markov chain or a continuous Markov process. The technique will be recognized as starting from the analog of a partition function but proved valuable in making the statistician aware of the extension of the notion of the characteristic function to the domain of Markov processes. Elliott showed that computations based on his technique could be expressed in terms of the properties of certain These could then be analyzed in terms of matrices. eigenfunction expansions of the relevant matrices. Among other benefits available with this technique is the possibility of finding Gaussian approximations as well as corrections to the calculated properties in a straightforward way, in contrast to more formal but somewhat less general techniques used in earlier mathematical literature.<sup>6</sup> This work also contained many of the recurring themes found in Elliott's

later work on stochastic processes and their applications. Elliott was a master of techniques involving applications of the asymptotic analysis of linear operators to problems in the physical sciences. The work described here was a significant contribution to applied probability.

Among Elliott's earliest work were three papers on lattice dynamics, a subject in which he became interested when working as a postdoctoral fellow with J. G. Kirkwood and in which he maintained an interest for many years following.<sup>8-10</sup> Until the time of Elliott's investigation, most of the work on thermodynamic properties of solids used the Debye model for the frequency spectrum of the solid in calculating these properties.<sup>11</sup> This model used the approximation that the frequency spectrum associated with a solid could be calculated from a continuum picture. It had been known since the work of Blackman in the 1930s that the Debye model was inadequate in reproducing much of the experimental data on the specific heat of solids. Blackman's work suggested that one could not neglect the lattice structure of the solid and suggested that the proper starting point for investigating thermodynamic properties of solids was the Born-von Karman model, which pictured the solid as a lattice of discrete atoms connected by springs that obeyed Hooke's law.<sup>12</sup> The question addressed in the first of Elliott's contributions to the subject was how to calculate the frequency spectrum for the Born-von Karman model.<sup>8</sup> The first step in the analysis consisted of showing that one could calculate moments in terms of the trace of powers of the dynamical matrix. The second step consisted of an expansion of the frequency spectrum in an infinite series of Legendre polynomials. In this way Elliott was able to reproduce many of the features of the frequency spectrum determined by Blackman by numerical

means. He later returned to the problem of doing exact two- and three-dimensional calculations of the frequency spectrum for simple cubic lattices using the Born-von Karman model, finding the infinite peaks later shown to be a general consequence of symmetry properties of the lattice.<sup>9,10</sup>

The theory of lattice dynamics proved to be a fertile field for Elliott's combination of techniques and talents for over twenty-five years dating from his initial contribution to this area of physics. As an example of this, Elliott and Renfrew Potts tackled the problem of calculating thermodynamic properties of lattices, particularly lattices with defects.<sup>13,14</sup> This involves computing sums of the form

$$S = \sum_{j} g(\boldsymbol{\omega}_{i}),$$

where  $g(\omega)$  is determined by the particular thermodynamic property and the  $\omega_j$  are the characteristic frequencies of the lattice determined by the solution of the dynamical equation  $D(\omega)=0$ , where  $D(\omega)$  is a determinant whose elements contain all of the physics of the problem. Montroll and Potts solved the problem very neatly by utilizing a representation derived from complex analysis

$$S = \frac{1}{2\pi i} \int g(z) \frac{D'(z)}{D(z)} dz$$

in which g(z) is the thermodynamic function, D'(z) is the derivative of the dynamical matrix, and the contour is chosen to surround the zeroes but not the poles of D(z). The effects of lattice defects could be found, using this formalism, by subtracting the contribution of the perfect lattice, which can be calculated in exactly the same way as indicated by the last equation.

Another significant finding contained in this particular series of papers is the technique for calculating the values of vibrational frequencies that may emerge from the con-

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tinuum of frequencies when defects are present in the lattice. Montroll and Potts showed that when there are ndefects in the lattice, a maximum of n frequencies will separate themselves from the continuum of frequencies found in the analysis of translationally invariant lattices. They further showed that the emergent frequencies could be found by the solution of an  $n \times n$  determinant whose elements consisted of Green's functions that characterize the lattice. All of the calculations were a demonstration of the elegance of essentially eighteenth-century classical mathematical analysis, of which Elliott was a master. Elliott's mastery of the subject of lattice dynamics led to his coauthorship of Lattice Dynamics in the Harmonic Approximation with Alex Maradudin and myself.<sup>15</sup> Somewhat characteristically, the book was originally supposed to have been a review article for Advances in Solid State Physics, which Elliott put off writing until there was so much material available that it could only fit into a book.

Aside from the analysis of lattice dynamic problems suggested by applications in solid state physics, Elliott, together with Peter Mazur, studied the properties of Poincaré cycles for an assembly of harmonic oscillators as a simple model for irreversibility in statistical mechanics.<sup>16</sup> This appeared in the first volume of the *Journal of Mathematical Physics*, of which Elliott was the founder and first editor. Because of Elliott's familiarity with the formalism on linear lattice dynamics, it was an easy and revealing tool for the analysis of problems that are quite difficult for physical systems with more complicated interactions. In the publication with Mazur, the authors were able to find precise results for the dynamics as expressed by the Poincaré cycle and the momentum correlation function. They were able to show that the length of the Poincaré cycle for a system of N atoms goes like exp(aN), the parameter *a* being positive, which identifies the time during which the system will appear to behave irreversibly.

While engaged in this work on lattice dynamics, Elliott also made fundamental contributions to the theory of unimolecular relaxation as a consultant to the National Bureau of Standards, in collaboration with Kurt Shuler.<sup>17,18</sup> The investigators managed to shed considerable light on an important field through the study of a simple physical model as well as to initiate lines of research in the study of chemical kinetics that have been pursued to the present time. Although the original work consisted of a study of the relaxation and dissociation of a weakly interacting system of harmonic oscillators, the formalism developed has been shown to apply to many other systems. The first step in this area of research was made by Landau and Teller, who calculated the collisional transition probabilities per collision for a system of harmonic oscillators, which subsequently allowed Bethe and Teller to find the average energy of an ensemble of such oscillators as a function of time. Montroll and Shuler first undertook the more exacting task of formulating a theory allowing the calculation of all of the statistical parameters characterizing the relaxation of the system. They did this by using Landau and Teller's form of the rate constants, which allowed them to write a master equation for the set of occupation probabilities of the different energy levels of the system. This system of equations could then be solved by using generating functions. Montroll and Shuler showed that the system of harmonic oscillators has the remarkable property that, if it has an initial Boltzmann distribution, it relaxes to its equilibrium Boltzmann distribution by means of a continuous sequence of Boltzmann distributions. It can be shown that the harmonic oscillator system is unique in this respect.<sup>19</sup>

Montroll and Shuler made a further significant advance using the harmonic oscillator model by adapting it to study the dynamics of the dissociation of diatomic molecules.<sup>18</sup> The simplifying feature of this model in a quantum-mechanical context is the fact that its energy levels are uniformly spaced. Montroll and Shuler studied the rate at which such a physical system reaches a critical energy of dissociation. In this way the analysis is framed in terms of the theory of first passage times. In this much-cited paper, the authors developed the theory of first passage times for the master equation, demonstrating its applicability to a physically interesting system. This work stimulated considerable further work, both on the mathematical theory of first passage times for master equations and on further applications of the formalism to other problems in chemical kinetics.

Perhaps the area with which Elliott's name is most closely associated is the theory and application of random walks. Elliott pioneered in the study of random walks on a lattice structure as opposed to random walks in a continuum, which had been the subject of most earlier investigations of the subject. This work grew out of Elliott's wartime study of the kinetics of cascades,<sup>20</sup> but it was also intimately related to his interests in solid state physics. A unifying thread throughout his many papers on this subject is the use of many of the same elegant mathematical tools he developed in his analyses of lattice dynamics. In one of his first papers on the subject, he tried to study the excluded-volume problem in polymer physics by analyzing properties of random walks with exclusions that only ranged over a fixed number of steps.<sup>21</sup> It is now known on general grounds that such a process remains Markovian and that one cannot hope to recover the non-Markovian properties that are characteristic of the excluded-volume random walk (e.g., the fact that the asymptotic mean square displacement of such a random walk varies with the number of steps, n, as  $n^{\alpha}$ , where  $\alpha \neq 1$ ). Elliott's first major contribution to the general theory of random walks was made some time later than his first essay into the area of the particular problems posed by the excluded random walk.<sup>22</sup> Most studies of random walk properties in the literature of the physical sciences had focused on random walks in a continuum. No doubt influenced by his work on lattice dynamics. Elliott developed the formalism necessary for the study of random walks on a lattice. Many of the mathematical tools developed in one context could profitably be carried over almost unchanged to the other. In addition, in this early work Elliott showed that Tauberian theorems for power series and Laplace transforms greatly simplified the calculation of many asymptotic properties of random walks. This work was taken up and extended somewhat later in Elliott's most cited paper.<sup>23</sup> A number of results scattered in the mathematical literature were derived in a unified manner by using Tauberian methods, but also a significant new model of lattice random walks was suggested in this paper allowing the notion of such walks in continuous time. In an earlier work, not directly related to random walks, Elliott developed what was essentially a theory of lattice walks in which the intervals between successive steps of the walk were allowed to be random.<sup>24</sup> However, since the distribution of these intervals took a specific form, the resulting random walk retained the Markov property, and there could be no basic difference between the properties of such random walks at very long times and those in which the times

between successive steps are constant. The so-called continuous-time random walk allowed for quite general distributions of interjump times.

Development of the theory of the continuous-time random walk was a purely theoretical one in Elliot's most frequently cited paper.<sup>23</sup> In another paper,<sup>25</sup> Harvey Scher and Elliott demonstrated some of the potentialities inherent in the formalism of the continuous-time random walk by applying it to anomalous dispersion arising in the transport of charge in amorphous solids. It was known at the time that photoconductivity experiments in certain classes of amorphous semiconductors, in which a pulse of light is applied to one face of the solid and a measurement is made of the carriers impinging on the second face, could not be explained in terms of a simple diffusion model. Scher and Montroll showed that the continuous-time random walk model could reproduce all of the peculiar qualitative experimental features observed provided that the probability density of interstep times has the property

$$\Psi(t) \sim t^{-(1+\alpha)}, 0 < \alpha < 1$$

at sufficiently large values of the time. This class of densities has the property of having no finite moments, which induces qualitative differences between such transport processes and ordinary diffusion processes since many of the mobile carriers tend to remain stationary for long periods of time. Somewhat later, Elliott, together with Michael Shlesinger, used related ideas in an attempt to explain the so-called Kohlrausch-Williams-Watt form for the dielectric relaxation function that frequently can be fit to data taken on polymers.<sup>26</sup>

Another area in which Elliott left an indelible mark, and

which is indicative of his wide-ranging and fertile imagination, is in the field of traffic flow. As a consultant to General Motors in the 1950s and early 1960s, Elliott became involved in and indeed was at the forefront of an effort to bring a more scientific approach to the characterization and control of traffic flow that had been initiated by Robert Herman. In a series of joint publications with Herman, Gazis, Rothery, Potts, and Chandler, Elliott developed the linear theory of car-following.<sup>27-29</sup> This theory relates the reaction of a driver in a single lane of traffic to the car in front of him. The simplest version of the theory is embodied in a set of equations for the speeds,  $v_j(t)$ , of a series of drivers, where  $j = 1, 2, 3, \ldots$ . These equations have the form

$$v_i(t) = \lambda [v_{i+1}(t-T) - v_i(t-T)],$$

where  $\lambda$  is a control parameter and T is the time for a driver to react to a change in relative speed. Using this greatly oversimplified model, which assumes that changes occur only in reaction to differences in relative speed, Elliott and his collaborators were able to show that for certain ranges in the two parameters,  $\lambda$  and T, a sufficiently long stream of traffic would tend to destabilize, leading to rearend collisions. This is indeed known to occur, for example, in foggy conditions where reaction times tend to be greater than normal. Later, Elliott extended the study of car-following equations by introducing the notion of "acceleration noise," represented by a random term added to the car-following equations written above. It was shown that the conditions leading to an instability in a line of cars also lead to an amplification of the noise. This work, which stimulated a large amount of further research by the traffic community, merited the award of the 1959 Lanchester Prize for Operations Research for Elliott, together with Chandler, Gazis, Herman, Potts, and Rothery.

This brief account of some of Elliott's work hardly begins to do justice to his wide-ranging interests, which included not only the physical sciences but also all aspects of the world around him. For example, Elliott, together with Robert Herman, wrote a paper on statistical properties of the prices found in Sears Roebuck catalogs over a period of years.<sup>30</sup> His interests in the history of science were legendary, and indeed his last published paper was on the ramifications and interconnections between scientific investigations initiated by nineteenth-century Viennese scientists.<sup>31</sup> Elliott also wrote papers on the denaturation of DNA,<sup>32,33</sup> model building in the biological and behavioral sciences,<sup>34</sup> as well as developing mathematical models to quantify technological development.<sup>35-37</sup> Few aspects of life or science escaped Elliott's attention. Elliott could be characterized as a Renaissance man transplanted into the twentieth century.

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