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Random Walks and Their Applications in the Physical and Biological Sciences

(NBS/La Jolla Institute, 1982)

Edited by
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American Institute of Physics

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DEDICATION

These proceedings are dedicated by his friends and colleagues to the memory of

ELLIOTT W. MONTROLL (1916-1983)

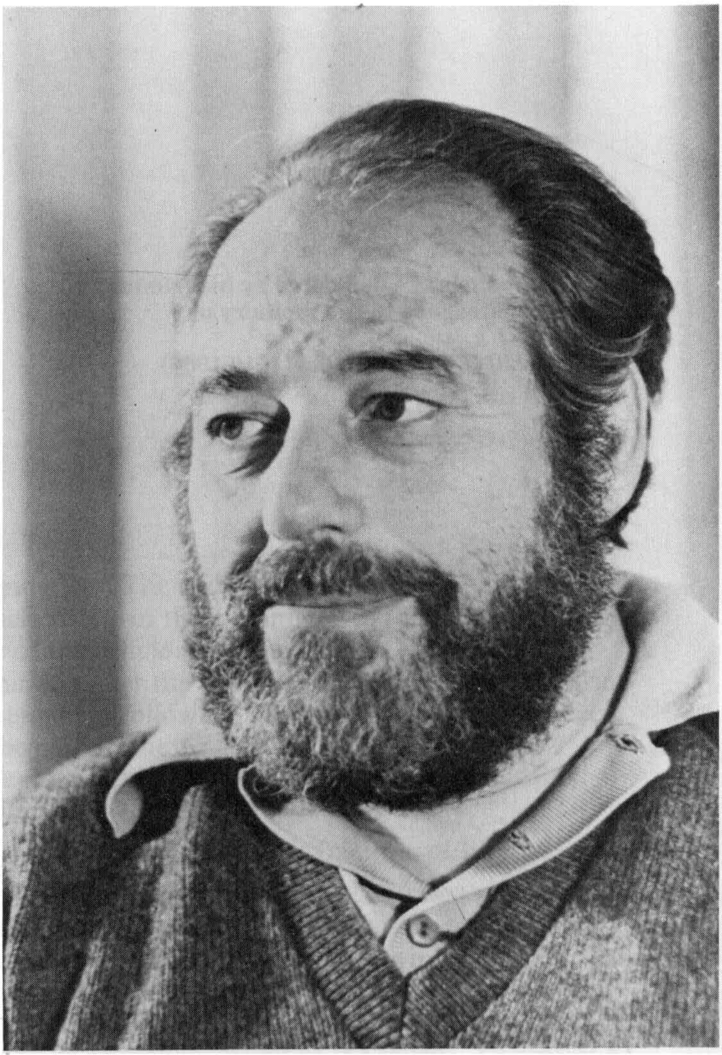

Photo courtesy of John Ward

ELLIOTT WATERS MONTROLL
(1916 - 1983)

ELLIOTT W. MONTROLL (1916-1983)
(In Memoriam)

Elliott Waters Montroll distinguished himself in many fields of science and mathematics while working in high-level positions at universities, the federal government, and in private industry. Some of his most outstanding achievements and most eloquent publications have been in the field of random walks, the topic of this proceedings which we dedicate to his memory. This work is briefly summarized below.

His article in this volume traces the influence of the Vienna School of Statistical Physics from Boltzmann to present day physicists, and includes the personage of Smoluchowski, a co-inventor of diffusion which is a form of a random walk. This complements a larger work of Montroll and Shlesinger [("On the Wonderful World of Random Walks," in *Studies in Statistical Mechanics, Vol. 11*, North-Holland Publishers (1984), in press] which reviews the history of random walks.

His first random walk encounter occurred while he was Head of the Mathematics Group of the Kellex Corporation (1943-1946). His task, connected to the Manhattan Project, was to design a stable control system for the cascade separation of two uranium isotopes at the Oak Ridge gaseous diffusion plant. His endeavor was highly successful. Part of the analysis involved the behavior of a third species which he found to obey a discrete space random walk (the state space being the levels in the cascade). The project was classified so he could not publish his result as such, but its mathematical version did appear as "A Note on Bessel Functions of Purely Imaginary Argument" in *J. Math. and Physics, Vol. XXV No. 1*, 37-48 (1946). He discovered that the generating function for a lattice random walk satisfies a Green's function equation which, in turn, also represents a lattice vibration problem. His pioneering work on lattice dynamics was published in the now classic book "Lattice Dynamics in the Harmonic Approximation" Academic Press (1963) with A.A. Maradudin and G.H. Weiss. Montroll's independent discovery of the random walk Feynman-Kac path integrals for quantum and classical mechanics can be found in the article "Markoff Chains, Wiener Integrals, and Quantum Theory" in *Comm. in Pure and Applied Math. Vol. V*, No. 4, 415-453 (1952).

Montroll and K. Shuler in "The Application of the Theory of Stochastic Processes to Chemical Kinetics" [(Adv. in Chem. Phys. Vol. 1, Interscience Pub. (1958)] discussed the shock induced dissociation of a diatomic gas as a random walk up and down a ladder of quantum mechanical energy levels. Dissociation occurs with the first passage to the uppermost level. The exact solution was obtained in terms of the little known Gottlieb polynomials.

Montroll's most quoted random walk paper is "Random Walk on Lattices II" with G.H. Weiss in *J. Math. Physics* **6**, 167 (1965). Here the generating function (Green's function) method is extended to include continuous-time processes. If the mean time between events is infinite the master equation approach to this problem fails, but E. Montroll, N. Kenkre, and M. Shlesinger in *J. Statistical Physics*, **9**, 45-50 (1973), showed that the random walk is equivalent to a generalized master equation.

These random walks with infinite temporal moments for the time interval between events provided the first successful explanation of charge transport in amorphous material such as xerographic films (see "Anomalous Transit-Time Dispersion in Amorphous Solids" by H. Scher and E.W. Montroll, *Phys. Rev.*, **B12**, 2455-2477 (1975). This analysis was later extended by E. Montroll and M. Shlesinger in "On the Williams-Watts Function of Dielectric Relaxation" *Proc. Nat.*

Acad. Sci. (USA) 1984 (in press) to model electric dipole relaxation in amorphous materials as a random walk controlled reaction process with relaxation occurring when a defect (e.g. a vacancy) reach a frozen dipole.

Two recent reviews of Montroll's random walk work are "An Enriched Collection of Stochastic Processes" by E.W. Montroll and B.J. West in "*Studies in Statistical Mechanics, Fluctuation Phenomena*, Chap. 2, (1979) and the earlier mentioned volume 11 of this series which besides the history of random walks includes work on fractal (self-similar) random walk paths.

Montroll was a Distinguished Professor at the Institute for Physical Science and Technology of the University of Maryland and a member of the National Academy of Science. He was an original in whose path many have followed. The impact of his work is apparent in the growth of random walk research evidenced by the international conference "Random Walks and Their Applications in the Physical and Biological Sciences." As with Lord Rayleigh whom he greatly admired, Montroll wrote his last papers on the topic of random walks.

Michael F. Shlesinger
Bruce J. West

PREFACE

In the past decade there has been an explosive growth in the theory and applications of random walks. The need for a meeting to bring together the leaders who have contributed to this surging growth was evident, and accordingly the conference "Random Walks and Their Applications in the Physical and Biological Sciences" was organized. It was held at the National Bureau of Standards from June 29 to July 1, 1982. The sponsors were:

National Bureau of Standards
National Institutes of Health
Exxon Research and Engineering Company
Xerox Webster Research Center
La Jolla Institute
Institute for Physical Sciences and Technology
of the University of Maryland

The Organizing Committee consisted of:

Robert Jernigan (NIH)
Joseph Klafter (Exxon)
Elliott W. Montroll (IPST, U. of Maryland)
Robert J. Rubin (NBS)
Harvey Scher (Xerox)
Michael F. Shlesinger (La Jolla Institute/IPST, U. of Maryland)
George H. Weiss (NIH)
Bruce J. West (La Jolla Institute)

The program of lectures is presented subsequently.

The study of fluctuations can lead to very powerful results and insights. Einstein's 1905 treatment of Brownian motion convinced reasonable minds of the existence of molecules and atoms by allowing Avogadro's number to be calculated from the second moment of a probability distribution.[1] While Einstein's physical interpretation of his Brownian motion was novel, much of the mathematics, unbeknownst to him, had been developed in 1900 by Bachelier[2] in a doctoral thesis (Poincaré headed Bachelier's thesis examination committee) devoted to price fluctuations in the stock market. Both men were studying a random walk process, the subject of this book. In the same period Smoluchowski, whose origins were in Vienna, was making important contributions to the theory of Brownian motion. The history of the Vienna school of statistical mechanics is reviewed here in an article by MONTROLL.

The first explicit mention of the words "random walk" appear in a 1905 query to the scientific community published in Nature by the great statistician Karl Pearson[3].

"A man starts from a point 0 and walks l yards in a straight line: he then turns through any angle whatever and walks another l yards in a second straight line. He repeats this process n times. I require the probability that after these n stretches, he is at a distance between r and $r + \delta r$ from his starting point 0. The problem is one of considerable interest, but I have only succeeded in obtaining an integrated solution for two stretches. I think, however, that a solution ought to be found, if only in the form of a series in powers of 1/n, where n is large."

Today this is called a Pearson or a Rayleigh-Pearson random walk because as Rayleigh pointed out in a reply to Pearson in Nature that he had solved this problem previously. Rayleigh[4] responded:

"The problem proposed by Prof. Karl Pearson in the current number of Nature, is the same as that of the composition of n isoperiodic vibrations of unit amplitude and of phases distributed at random, considered in Philosophical Magazine X, p. 73, 1880; XLVII, p.246, 1889. If n be very great, the probability sought is

$$2n^{-1} exp(-r^2/n)\, rdr \quad .$$

Probably methods similar to those employed in the papers referred to would avail for the development of an approximate expression applicable when n is only moderately great."

KIEFFER and WEISS treat further developments in the analysis and application of the Rayleigh-Pearson random walk. They discuss applications and develop approximations for the probability density function for end-to-end distances and projections on an axis. In 1934, Kuhn[5] characterized polymer chain configurations in terms of these random walks, but this neglects volume exclusion effects. Modern techniques using a real space renormalization group to study polymer statistics is presented here by FAMILY. An analogy is made between critical phenomena when $T \to T_c$ and polymer statistics as the number of monomers $N \to \infty$. Family categorizes the universality of polymer models and analyzes the crossover behavior between them. RUBIN reviews and further advances the investigation of the absorption of an isolated polymer chain at a solution surface. Each random polymer configuration corresponds to a self-avoiding random walk on a lattice. The random walk paths can be weighted to favor sticking to the solution surface. A critical weighting is found which leads to an absorption -desorption transition. A comparison is made to a similar model involving polymer configurations near a reflecting surface.

Of course, random walks by other names, go back far beyond Pearson, at least to Jacob Bernoulli's posthumously published treatise of 1713 *Ars Conjectandi.*[6] He described what is now called a Bernoulli process: In a sequence of independent trials, success occurs with probability p and failure with probability q=1-p. The number of successes fluctuates in an manner equivalent to a random walker on a lattice with probabilities p and q for moving forward or backward. Bernoulli's gambler's ruin problem is equivalent to a random walk on a lattice between two absorbing boundaries. This work was a generalization of Huygen's investigations of gaming odds in his 1657 treatise *De Ratiociniis in Ludo Aleae*[7], which in turn was motivated by the Pascal-Fermat correspondence of 1654 on games of chance. Bernoulli calculated the probability of m successes P_m in n trials to be

$$P_m = \frac{n!}{m!\,(n-m)!} p^m q^{n-m} \quad (1)$$

De Moivre[8] in his *The Doctrine of Chances* of 1735 showed that eq. (1) tends to a Gaussian distribution centered around n/2 when p=q. This is 76 years before Gauss' publication of the Central Limit Theorem which applies to this and also more general cases.

That the study of random walks does not end with Gaussian probability distributions was realized early on as exemplified by Daniel Bernoulli's 1731 discussion of the Petersburg Paradox (apparently receiving this nomenclature because it was published in the Comentarii of Petersburg Academy[9]). The Paradox involved calculating the "fair" entrance fee for playing a particular Bernoulli process: Flip a coin, if a head appears, win one penny, if a tail appears, flip the coin again. Repeat the process until a head appears. If a head appears for the first time on the nth trial, win 2^{n-1} pennies. The probability p_n of winning 2^{n-1} pennies is 2^{-n}, thus the expected winning is

$$\sum_{n=1}^{\infty} 2^{n-1} p_n = \infty \; . \quad (2)$$

Now suppose you want to play this game against a bank with an infinite reserve of money, how much money would you stake just because your *expected* winning is infinite? You would hesitate to wager a large amount because your *median* winning is only one penny. Thus, the paradox is should your intuition follow the mean or the medium? It is fascinating that such questions come into play again in recent times concerning the random walk of charges in highly disordered environments such as xerographic films. Currents can be generated in the presence of an electric field because the *median* time for a charge to jump is finite, but because the *mean* time between jumps is infinite the currents are only transient.

The general theory of the limiting forms of probability distributions which are not Gaussian was discovered by Paul Lévy[10] and was called by him the theory of stable distributions. These are distributions for a sum of identically distributed random variables where the sum and any one of its terms have the same distribution except for scale factors. The Cauchy distribution is one such example. All of these distributions have their second or a lower (possibly non-integer) moment being infinite. They thus have long tails, no characteristic size in which to gauge measurements, and describe self-similar behavior. Random walks in the continuum with jump length distributions of the Lévy type (infinite second moments) are called Lévy flights. Their trajectory has a fractal dimension in the sense of Mandelbrot[2] (Lévy's protegé). HIOE'S article relates correlation functions for Lévy flights on a lattice to spin correlation functions for the spherical model of ferromagnetism with long-range interactions.

The most famous paper on lattice random walks is Polya's[11] proving that a random walker taking nearest neighbor jumps on a periodic, infinite cubic type lattice will only return to its starting point in two or less dimensions. The precise probability for not returning on various three dimensional lattices was first calculated by Montroll.[12] Starting in the 1940's Montroll has contributed much original work and many clear expositions to the theory of random walks. His Green's function and generating function techniques have made random walk theory accessible to the physics community. Many lecturers at this conference can trace their random walk roots back to Montroll. His classic 1965 work with George Weiss on continuous-time random walks[13] (CTRW) has been the cornerstone for many theories of transport in condensed matter. Lindenberg, Heminger, and Pearlstein[14] treated exciton transport in molecular solids as a random walk with randomly placed traps, using Montroll's techniques. In addition, they accounted for the possible trap configurations via the coherent potential approximation. The article by WEST and LINDENBERG treats exciton migration at finite temperatures. Previous theories were essentially infinite temperature models. West and Lindenberg add the proper dissipation term to their Hamiltonian equation of motion so the system can reach thermal equilibrium. This allows them to calculate, for the first time, the temperature dependence of quantities such as exciton lineshapes.

The growth in the interest in random walks has in part been due to the calculations of P.W. Anderson[15] showing that electronic wave functions can be localized in a sufficiently random environment. In this spirit, using the Montroll-Weiss walk to calculate a quantum-mechanical probability Scher and Lax[16] in 1973 analyzed the frequency dependent conductivity of impurity conduction of doped semiconductors. The article by LAX and ODAGAKI continues this field of research by treating more accurately the random walk in a random media. The multiple scattering theory of Lax is used to derive a coherent medium approximation for the hopping of charges in a random media. Dynamic percolation is automatically included in the calculation.

SCHER and RACKOVSKY'S article extends the earlier random walk transport model to geminate recombination of charge pairs. The Colomb field of the charges as well as the effect of an external electric field are taken into account. The random walk Green's function approach includes defective sites and allows the effects of dimensionality, disorder, tunneling, and intramolecular transitions to be analyzed exactly.

Scher and Montroll[17] were the first to treat the transient currents in xerographic films as a random walk process governed by a waiting time distribution between jumps which has an infinite mean. The connection of these processes to fractal times, Lévy distributions and renormalization groups has been explored by Shlesinger and Hughes.[18] Reaction schemes governed by this fractal time process for electron-hole recombination in an inhomogeneous environment is the subject of the article by KLAFTER and BLUMEN.

Random walks need not take place in a real positional space and the transitions need not represent actual physical jumps. Many problems can be mapped exactly onto a random walk problem, although the appropriate random walk may be semi-Markovian, non-Markovian, involve internal states, memories, a high number of dimensions, a defective lattice, difficult boundary conditions, or other complications. For example SAHIMI, in his article is able to treat flow paths through a random network as a continuous-time random walk. Percolation effects are also included, with information about the structure of the percolation backbone being derived from the dispersion of the flow.

While there has been much attention paid to the behavior of a single particle in a random potential, a more difficult question involves the dynamics of a fluid in a random potential. MUKAMEL, in his article, addresses this issue and calculates the conductivity and density function response of the fluid as these are experimentally observable quantities.

In the last article CLAY and SHLESINGER describe the passage of potassium ions through a channel in a neural membrane in terms of a random walk model whose internal states represent the contents of the channel. The kinetics of gates which can block the current are included in the analysis. Modifications of the Hodgkin-Huxley equations for the gating process are proposed. The model leads to exact results which can be used to analyze flux experiments.

We wish the reader much enjoyment with this volume. For those who find random walks irresistible we suggest the following reviews:

1. M. Barber and B. Ninham, *Random and Restricted Random Walks* (Gordon and Breach Pub. NY) 1970. This is a fairly complete review of the already extensive random walk literature up to 1970.

2. M.F. Shlesinger and V. Landman, in *Applied Stochastic Processes*, G. Adomian ed. (Academic Press, NY) 1980, p. 151-246. Treats many problems which can be cast as random walks with internal states.

3. E.W. Montroll and B.J. West, in Studies in Statistical Mechanics, **VII**, *Fluctuation Phenomena* eds. J.L. Lebowitz and E.W. Montroll, (North-Holland Pub.) 1979, p. 61-175. Good review of continuous-time random walks, boundary and defect problems, Lévy distributions, first passage time distributions, and nonlinear diffusion processes.

4. G.H. Weiss and R.J. Rubin, in Advances in Chemical Physics, **52**, eds. I. Prigogine and S.A. Rice (John Wiley & Sons Inc., N.Y.) 1983, p 363-505. A good recent review of general theory and applications to polymer physics, multistate random walks, solid state physics, and motion of micro-organisms.

5. E.W. Montroll and M.F. Shlesinger, in CCNY Physics Symposium in Celebration of Melvin Lax's 60th Birthday, H. Falk ed., (CCNY Physics Dept., NY) 1983, p. 44-147 and E.W. Montroll and M.F. Shlesinger in Studies in Statistical, **11**, *Nonequilibrium Phenomena 11* eds. J.L. Lebowitz and E.W. Montroll, (North Holland Pub) (in press). The emphasis is on the history of probability theory and the theory and applications of fractal random walks.

6. Journal of Statistical Physics **30** No. 2 (1983). Eds. G.H. Weiss and R.J. Rubin. Contains twenty-nine papers presented at the Random Walks in the Physical and Biological Sciences conference. Full of good research problems.

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PROGRAM

A history of stochastic processes.
Elliott W. Montroll, University of Maryland
From classical dynamics to continuous time random walks.
Robert Zwanzig, University of Maryland
Random walk model for 1/f noise.
Mark Nelkin, Alan Harrison, Cornell University
Diffusion in random one-dimensional systems.
W. Schneider, J. Bernasconi, Brown Boveri Research Center
Diffusion and relaxation in disordered systems.
B. Movaghar, Hirst Research Center
Multiple scattering, CPA, and CTRW treatment of hopping conductivity.
Melvin Lax, T. Odagaki, City University of New York and Bell Laboratories
Analytic continuation method for estimating effective parameters for multicomponent random walks.
George Papanicolau, Courant Institute
Random walks on inhomogeneous lattices.
P. W. Kasteleyn, W. Th. F. den Hollander, University of Leiden
Laser speckle as a two-dimensional random walk.
Richard Barakat, Harvard University
A random walk model of multiphase dispersion in porous media.
Muhammad Sahimi, L. E. Scriven, H. T. Davis, University of Minnesota
Random walks and renormalization theory: The central limit theorem as a fixed point.
P. B. Visscher, University of Alabama
Nonexponential decay in relaxation phenomena.
A. K. Rajagopal, Louisiana State University; K. L. Ngai, R. W. Rendell, S. Teitler, Naval Research Laboratory
From random to self-avoiding walks.
Cyril Domb, Bar-Ilan University
Self-avoiding walks with geometrical constraints.
S. G. Whittington, University of Toronto
Stochastic processes originating in deterministic microscopic dynamics.
Joel Lebowitz, Rutgers University
Stochastic flows in integral and fractal dimensions and morphogenesis.
John J. Kozak, University of Notre Dame
Stochastic stick boundary conditions.
Irwin Oppenheim, Massachusetts Institute of Technology; N. G. van Kampen, Rijksuniversiteit Utrecht
Stochastic aspects of biological locomotion.
Ralph Nossal, National Institutes of Health
Phase transitions in a four-dimensional random walk with application to medical statistics.
Ora E. Percus, Jerome K. Percus, Courant Institute
Protein folding as a random walk.

Nobuhiro Go, Kyushu University

Conformational space renormalization group treatment of polymer excluded volume.

Karl Freed, James Franck Institute

Cell renormalization for self-avoiding random walks and lattice animals.

Fereydoon Family, Emory University

Single and multiple random walks on random lattices: Excitation trapping and annihilation simulations.

R. Kopelman, P. Argyrakis, J. Hoshen, J. S. Newhouse, University of Michigan

Correlation factors for diffusion via the vacancy mechanisms in crystals.

Masahiro Koiwa, Shunya Ishioka, Tohoku University

Diffusion in concentrated lattice gases.

Klaus W. Kehr, Institut fur Festkorperforschung

Random walks on random lattices with traps.

V. Halpern, Bar-Ilan University

Energy transfer as a random walk with long-range steps.

Alexander Blumen, Technische Universität; G. Zumofen, ETH-Zentrum

Rotational diffusion in solid polymers.

J. T. Bendler, General Electric

On the mean motion and some statistical properties of quasi-periodic observable in a fermion-boson model.

F. T. Hioe, University of Rochester

Monte Carlo renormalization group calculation for polymers.

H. Muthukumar, Illinois Institute of Technology

Trapping of excitation in the average T-matrix approximation.

D. L. Huber, University of Wisconsin

Diffusion-controlled reactions.

R. Cukier, Michigan State University

Transport processes in disordered solids.

Kurt E. Shuler, University of California, San Diego

Equilibrium folding and unfolding pathways for a model protein.

Robert L. Jernigan, S. Miyazawa, National Institutes of Health

Physics of migration of ligands in biomolecules.

Peter Hanggi, Polytechnic Institute of New York

Master equation techniques for exciton motion, capture, and annihilation.

V. M. Kenkre, University of Rochester

Random walk to and interaction with an impurity.

Peter M. Richards, Sandia National Laboratory

Monte Carlo simulation of electronic transport in disordered media.

M. Silver, University of North Carolina; H. Baessler, G. Schoenherr, Universitat Marburg; Leon Cohen, Hunter College

Renormalization group approach to random walls on disordered lattices.

Jonathan Machta, University of Maryland

On the dynamics of excitations in disordered systems.

S. Mukamel, Weizmann Institute of Science

Approach to asymptotic diffusive behavior in strongly disordered lattices.