

Genesis of the Monte Carlo Algorithm for Statistical Mechanics

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I fear that 50 years is a bit long for expecting much from the originators of the first applications of a technique. Mici Teller and Nick Metropolis are dead. Edward Teller and Arianna Rosenbluth are too infirm to travel. It is not easy for me either, but in the hope of learning something about the last 50 years of progress from our crude beginnings, I am glad to be here, and I will try to give you my subjective history of the development and motivations of the first papers on the topic.

The period 1949-1952 here at Los Alamos 50 years ago was of course a time of great excitement as the successful concept for a hydrogen bomb had been proposed by Teller, and was being fleshed out by the members of the small theory group. We worked 60 hours or more per week trying to understand the physics of the interactions of radiation and matter under these extreme conditions, and how the explosion/implosion/ explosion would evolve. A key issue was of course the equation of state which was the origin of my interest in the subject. At this time the first electronic computers were just coming into being, and until the end of 51 the work was mainly analytic, supplemented by some implosion codes on the punchcard IBM machines. Nonetheless by this time our crude results, supplemented by the successful Greenhouse tests, led to a high degree of confidence that the Mike shot in Nov.52, the first HBomb, would succeed, in fact was quite overdesigned. Still as the new computers finally came on line it was obviously necessary to do the most detailed possible calculations .For the next few months my first wife, Arianna, and I devoted ourselves to this task and she in particular became one of the first and most skillful adepts at this new game.

Let me recall the state of computers in those days. The driving force in the US was of

course John von Neumann, or Johnnie as everyone called him. Aided by Herman Goldstein, Julian Bigelow, and others, a machine, the Johnniac was being built at the Institute for Advanced Study in Princeton. It was motivated primarily by HBomb design. A copy, the MANIAC, was being built here at Los Alamos, under the engineering supervision of Jim Richardson .. For whatever reason the radically new Princeton and Los Alamos machines came into operation just too late for Mike design, so Arianna and I went to the SEAC, a similar machine, and the first true electronic computer, which had just gone into operation at the Bureau of Standards in Washington. Here we became accustomed to months of midnight shift existence. In the event the SEAC work confirmed our analytic predictions and we decided to look for new science which could exploit the now operational MANIAC.

The heart of the MANIAC was 1024 vacuum tubes. These served to execute the logic , to store the program, and as fast access storage for calculational quantities. Compare this with the many megabyte RAM of present PCs. Slow access memory was also available on magnetic tapes. As best I recall multiply times and various logic and access orders took of the order of 100 microseconds each. Again performance, while phenomenally better than what was available a few years earlier, was pathetic by today's standards. Programming was in assembly language, similar to BASIC.

Considering the possibilities, Arianna and I with Tellers encouragement, decided that many body systems offered an important application inaccessible to analysis, but possibly compatible with MANIACs abilities. In particular the liquid-solid transition was, and for all I know, still is mysterious. Why did the change from a close-packed array in which nearest neighbors were fixed, to a regime where molecules slipped past each other occur via a discontinuous first order phase transition? Was an attractive force between molecules essential or would rigid spheres exhibit the same behavior? Was it a 2 or 3 dimensional phenomenon? So we decided to investigate the equation of state of rigid spheres, at first in 2 and later in 3 dimensions.

We then secured, with Teller's help, Metropolis' agreement to let us have the midnight shift on the MANIAC as long as it was not needed for other projects. Fortunately, the

machine had few demands on it at that time and was operational about half the time so that Arianna and I had a lot of running time.

Of course our first thought was straightforward molecular dynamics, following the motion of our collection of several hundred particles as they moved in time. As we considered the requirements for doing this, it was soon obvious that very small time steps would be required to accurately follow the dynamics of all the interacting particle pairs, and to consider the detailed kinematics of collisions. It looked impossible to use an adequate number of particles with the MANIACS limited capabilities. At this point Teller came up with THE crucial suggestion: since we were interested only in equilibrium quantities we should take advantage of statistical mechanics and take ensemble averages instead of following detailed kinematics.

This started me thinking about the generalized Monte Carlo approach about which I had talked often with von Neumann. The basic idea, as well as the name was due to Stan Ulam originally, and very simple-that in many complex situations it was not necessary to consider all possible trajectories but only to look at a large, random sampling of them. This approach of course only works if one has a sufficiently powerful computer. By 1952 some Monte Carlo tracing of neutrons and photons as they changed energy and moved in complicated structures had already been implemented at LANL. The location and outcome of scattering and absorption events was determined by comparison with a computer-generated random number. This application was discussed in papers by Everett and Ulam and Metropolis and Ulam in the late 40s . Goldberger ,at Fermis suggestion, did a hand (!) MC calculation of neutron interactions with nuclear matter, following about 100 tracks. This technique is of course now widely employed in particle physics to analyze tracks and is the basis of particle-in-cell hydrodynamic, magnetohydrodynamic, and kinetic astrophysical and plasma applications. Parenthetically I might mention that in these latter applications the particles are sources for the fields, and there seems as yet no adequate understanding of convergence and error build up.

As Johnnie had pointed out to me, the technique was more general and could be employed to evaluate many dimensional integrals by choosing a random , properly weighted, selection

of points. With an N -dimensional grid with y grid points per dimension one would require y^N points to do a classic evaluation of the integral, while a Monte Carlo approach with a million or so points would probably suffice. So, clearly for high dimensional integrals the MC approach was indicated. I noted that taking an ensemble average for a system of several hundred particles was indeed a $d * N$ dimensional integral (with d the number of space dimensions.) For the canonical ensemble one needed to evaluate ensemble averages with all possible configuration space points weighted with a factor $\exp(-E/T)$.

Again the most obvious approach, placing the particles in random positions to generate a point of the ensemble, could not work since one would overwhelmingly select points of very low a priori probability with some pairs of particles very close together. It was clearly necessary to devise a scheme which would allow our ensemble point to move through phase space avoiding regions of low probability. By analogy with molecular dynamics, the obvious approach was to make a pseudo move and check the energy change induced by it. Hence the pseudomoves represent, not a motion in time, but a generation of suitable configurations in the ensemble.

The outline of the approach was now clear. Make an a priori pseudomove which conserved phase space (note that with the classical canonical ensemble the velocity space integrals are trivial). The move could involve one, several, or many particles. Hence a 1 particle move to a random position within a square or sphere of given size around the initial position would satisfy this requirement as long as the reverse a priori move was equally probable and the procedure was ergodic. Then insure that the ratio of the probability of the moves in either direction is given by $\exp(\Delta E/T)$ with ΔE the energy difference between the 2 states.. A simple way to do this, as emerged after discussions with Teller, would be to make the trial move: if it decreased the energy of the system, allow it,- if it increased the energy allow it with a probability $\exp(-\Delta E/T)$ as determined by a comparison with a random number. Each step, after an initial annealing period, is counted as a member of the ensemble, and the appropriate ensemble average of any quantity determined.

We illustrate the algorithm for the trivial case of a 1D system with 2 particles (see Fig.

1). The state of the system is represented by (x_1, x_2) . For example the computation may be in the state shown by the centroid of the dotted cross. The algorithm would then tell us to make an a priori move with equal probability to any point along one of the dotted line segments. Following this we would determine the energy change, in this case dependent on $(x'_1 - x'_2)$. The algorithm would then tell us if the move were to be allowed or if the system remained in its present state. For hard disks the hatched region near the diagonal would be forbidden. Thus the system moves through the phase space, spending the canonical fraction of its time in each volume. Hence the ensemble average of any quantity, such as the energy can be obtained by averaging it over many moves of the system.

The most important property of the algorithm is that not only is the canonical distribution a steady state solution but that an analog of the Boltzmann H Theorem is valid, so that deviations from the canonical distribution die away. Hence the computation converges on the right answer! I recall being quite excited when I was able to prove this.

Let P_ν^N be the ensemble probability that the system is in the state ν after the N th move. Here for convenience we replace the $3N$ dimensional configuration space volume element by state ν . Then the algorithm tells us after the $N + 1$ move the probability distribution has evolved to:

$$P_\nu^{N+1} = \sum_{E_{\nu'} > E_\nu} P_{\nu'}^N T_{\nu'\nu} + \sum_{E_{\nu'} < E_\nu} P_{\nu'}^N T_{\nu'\nu} e^{-\frac{|\Delta E_{\nu\nu'}|}{T}} + P_\nu^N \sum_{E_{\nu'} > E_\nu} T_{\nu\nu'} (1 - e^{-\frac{|\Delta E_{\nu\nu'}|}{T}}) \quad (0.1)$$

Here $T_{\nu\nu'}$ is the a priori probability for moving from state ν to state ν' . Note $T_{\nu\nu'} = T_{\nu'\nu}$ and $\sum T_{\nu\nu'} = 1$. The probability at $N + 1$ is composed of 3 components: moves from states ν' of higher energy, moves from states of lower energy, and a component from moves which were forbidden so the system remains in state ν . Note that it is crucial to retain these. Several properties are trivially shown. Probability is conserved and the canonical distribution $P_\nu = e^{-\frac{|\Delta E_{\nu\nu'}|}{T}}$ is indeed a steady state. To proceed to the H theorem it is useful to put the evolution equation into Sturm-Liouville form. This is most conveniently done by introducing new variables $P_\nu = D_\nu * X_\nu$, with $D_\nu = \exp(-E_\nu/T)$. Then:

$$D_\nu(X_\nu^{N+1} - X_\nu^N) = \sum_{E_{\nu'} > E_\nu} D_{\nu'} T_{\nu\nu'} (X_\nu' - X_\nu) - \sum_{E_{\nu'} < E_\nu} D_\nu (X_\nu' - X_\nu) T_{\nu\nu'} \quad (0.2)$$

We can then expand in eigenmodes $X_j(N+1) = \lambda_j * X_j(N)$. Orthogonality is easy to prove i.e. $(x_j D x_{j'}) = 0$. Further:

$$(\lambda_j - 1) \sum X_{\nu,j} D_\nu X_{\nu,j} = - \sum_\nu \sum_{E_{\nu'} > E_\nu} D_{\nu'} T_{\nu\nu'} (X_\nu' - X_\nu)^2 \quad (0.3)$$

Hence all eigenvalues fall in the range $1 > \lambda > 0$. Only X_ν independent of state, i.e.the canonical distribution has $\lambda = 1$. Thus we can expand any initial distribution into eigenstates and after many moves all but the canonical will have died away, thus proving the H theorem. Equation 0.3 is also of some guidance in optimizing move strategies ,although convergence rates and fluctuation levels are best determined by numerical experimentation.

After Arianna had ably coded the algorithm up within the limits imposed by machine capability, we found that the algorithm was robust, worked remarkably well, and no real unexpected problems turned up. Of course various tricks were incorporated such as starting at high temperature to reach the equilibrium more quickly and using periodic boundary conditions to increase the effective number of particles.

For our purposes we calculated the 2 particle radial distribution function, from which the pressure can be determined by means of the virial theorem.. To briefly remind you of the virial theorem. Start from the equation of motion of the ith particle. X_i'' is due to the force exerted by the other particles and the pressure from collisions with the wall. Multiply by X_i and sum over all particles:

$$\sum_i m_i \vec{X}_i \cdot \ddot{\vec{X}}_i = \frac{d^2}{dt^2} \sum_i m_i \frac{\dot{\vec{X}}_i^2}{2} - \sum_i m_i \dot{X}_i^2 = -\frac{1}{2} \sum_{i,j} \frac{\delta V}{\delta r_{ij}} r_{ij} - PA \quad (0.4)$$

Hence the pressure is determined by the ensemble average of the virial: $\sum(\text{all pairs}) r * dV/dr$. This we get from the 2 particle radial distribution function of our Monte Carlo run. For the particular case of hard disks of radius r_o this reduces to:

$$PA = NT(1 + 2\pi r_o^2 \tilde{n}) \quad (0.5)$$

with \tilde{n} the value of the radial distribution function at $r_1 - r_2 = 2r_o$ when the disks are just touching.

Let me now discuss very briefly the 50 year old physics of our results. For the 2D rigid disks, as the density is decreased the configuration changes gradually from a well-ordered lattice to a more or less chaotic distribution. As I remember we were able to run with several hundred particles. At high and low densities our results fit well with the approximate theories- excluded volume at high densities, an improved virial expansion at low. We also were able to calculate new terms in the virial expansion by Monte Carlo evaluation of the cluster integrals. Of key interest was the intermediate region where one could have expected a possible phase transition. In fact it turned out that the equation of state curve showed no discontinuities (see Fig. 2) It required many runs, including different initial states and move algorithms, to convince us this was the case. The statistical errors, after many nights of operation, were very small. Going on to 3 dimensions the results were similar-no phase transition. One unexpected feature was that the peak of the radial probability occurred away from the touching point. I don't believe there is a theoretical explanation but this has been observed experimentally in neutron scattering from liquids (see Fig. 3).

Next we moved on to the Lennard-Jones potential. $V = a * r^{-12} - b * r^{-6}$. In stark contrast with the rigid sphere case the equilibrium showed a clear coexistence of 2 phases. (see Fig. 4). Unfortunately the MANIAC's capabilities did not allow for a quantitative equation of state in the transition region. The large surface area between phases and high fluctuation levels precluded this. Nonetheless the qualitative features were clear.

Let me finally just mention 2 applications which we studied as random walk problems, although not using exactly the same algorithm. A simple model for a polymer is a random walk chain in which previously occupied sites are forbidden. The question we considered is how the geometric length of the chain varied with the number of sites. Of course for an unrestricted random walk $L = N^{0.5}$. For our restricted walk we found $L = N^{0.61}$. As I recall previous analytic approximations gave exponents $0.67 - 0.75$.

A more exacting project, which never got beyond a very preliminary exploratory stage was to calculate the equilibrium at zero temperature of a Bose-Einstein liquid such as 4He . Here we exploited the fact that the $3N$ dimensional Schrodinger equation has the same

form as the neutron diffusion equation (in $3N$ dimensions) with a fission or absorption rate proportional to the potential energy. This diffusion system can be advanced in imaginary time through the Monte Carlo scheme for neutron transport discussed earlier. Since the lowest energy state should be symmetric the statistics would automatically be Bose-Einstein. The eventual growth rate of the wave function is equal to the ground state energy. The minimum as a function of density gives the predicted liquid density. Our results were never satisfactory enough to publish, since we could keep only a few atoms and fluctuations were large.. However we found that with the Lennard Jones potential we could get a reasonable result for the ground state density of 4He . We then calculated 3He as if it were a Bose gas and determined that the difference in masses could only account for about half the observed density difference, the rest presumably being due to the fact that 3He really obeys FermiDirac statistics . I was never able to think of a MonteCarlo method for properly treating a FermiDirac system. Obviously we had hardly scratched the surface of the quantum Monte Carlo problem.

By 1954, I had been introduced by Jim Tuck to the intricacies of controlled fusion and plasma physics to which I have devoted the rest of my professional life. I regret to say that I have not followed all the amazing work on the Monte Carlo method which has been done in the meanwhile. Hence I am keenly curious to get some sense of it at this meeting. I must confess that while at the time I felt our work to be satisfying and exciting and maybe even important, I could never have imagined that it would still be remembered 50 years later.

It gives me great pleasure to visit Los Alamos again and think of that era. The aura of scientific optimism here in those days was a wonderful tonic for a new PhD. Especially the chance to interact with great minds like John von Neumann and Edward Teller (see Fig. 5) provided an unparalleled education. Of course the opportunity to be in the right place at the birth of the age of the computer was a wonderful piece of luck. I am happy to know that Los Alamos, thanks in part to the leadership efforts of Nick Metropolis, has remained all these years in the forefront of scientific computing.

FIGURES

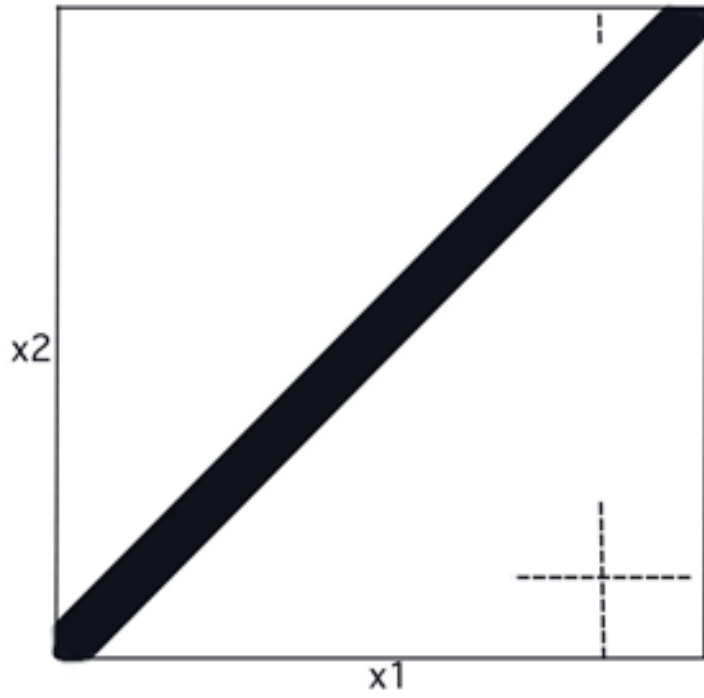


FIG. 1. Schematic of an ensemble point.

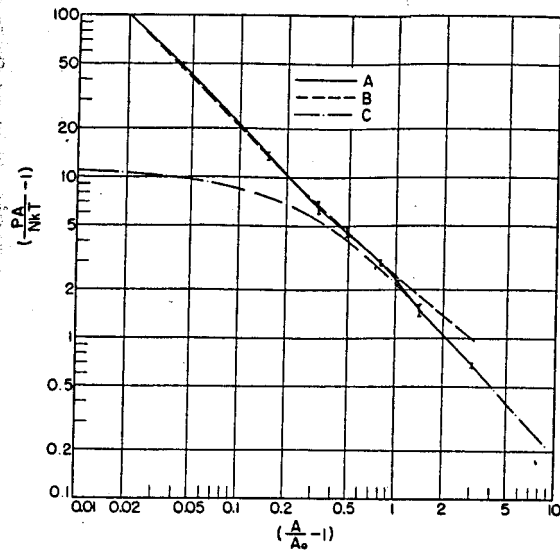


FIG. 2a A plot of $(PA/NkT) - 1$ versus $(A/A_0) - 1$. Curve A (solid line) gives the results of this paper. Curves B and C (dashed and dot-dashed lines) give the results of the free volume theory and of the first four virial coefficients, respectively.

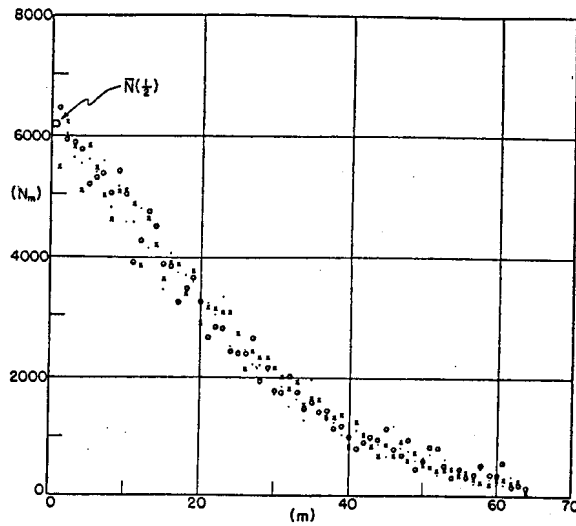


FIG. 2b The radial distribution function N_m for $\nu=5$, $(A/A_0) = 1.31966$, $K=1.5$. The average of the extrapolated values of N_1 in $N_1 = 6301$. The resultant value of $(PA/NkT) - 1$ is $64N_1/N^2(K^2 - 1)$ or 6.43. Values after 16 cycles, \bullet ; after 32, \times ; and after 48, \circ .

FIG. 2. 2D hard sphere results.

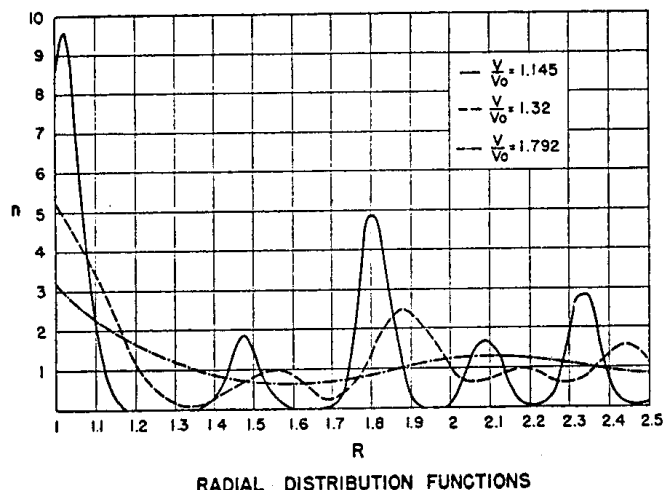


FIG. 3a Radial distribution functions *versus* distance for three-dimensional hard spheres. Here n , the density of molecules surrounding a given molecule, is normalized to one for a uniform distribution. The distance R is given in units of the molecular diameter. Distribution functions for three volumes are shown.

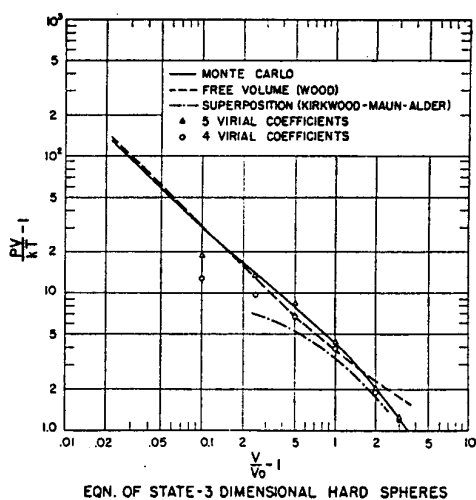


FIG. 3b A log-log plot of $(PV/kT) - 1$ *versus* $(V/V_0) - 1$ for hard spheres in three dimensions. Here V_0 is the volume per molecule at the closest possible packing. The solid line is the result of the Monte Carlo method as discussed in this paper; as compared to the free volume theory (dashed line), the superposition theory of Kirkwood (dot-dashed line), and to a 4 term (circles) and 5 term (triangles) virtual expansion.

FIG. 3. 3D hard sphere results.

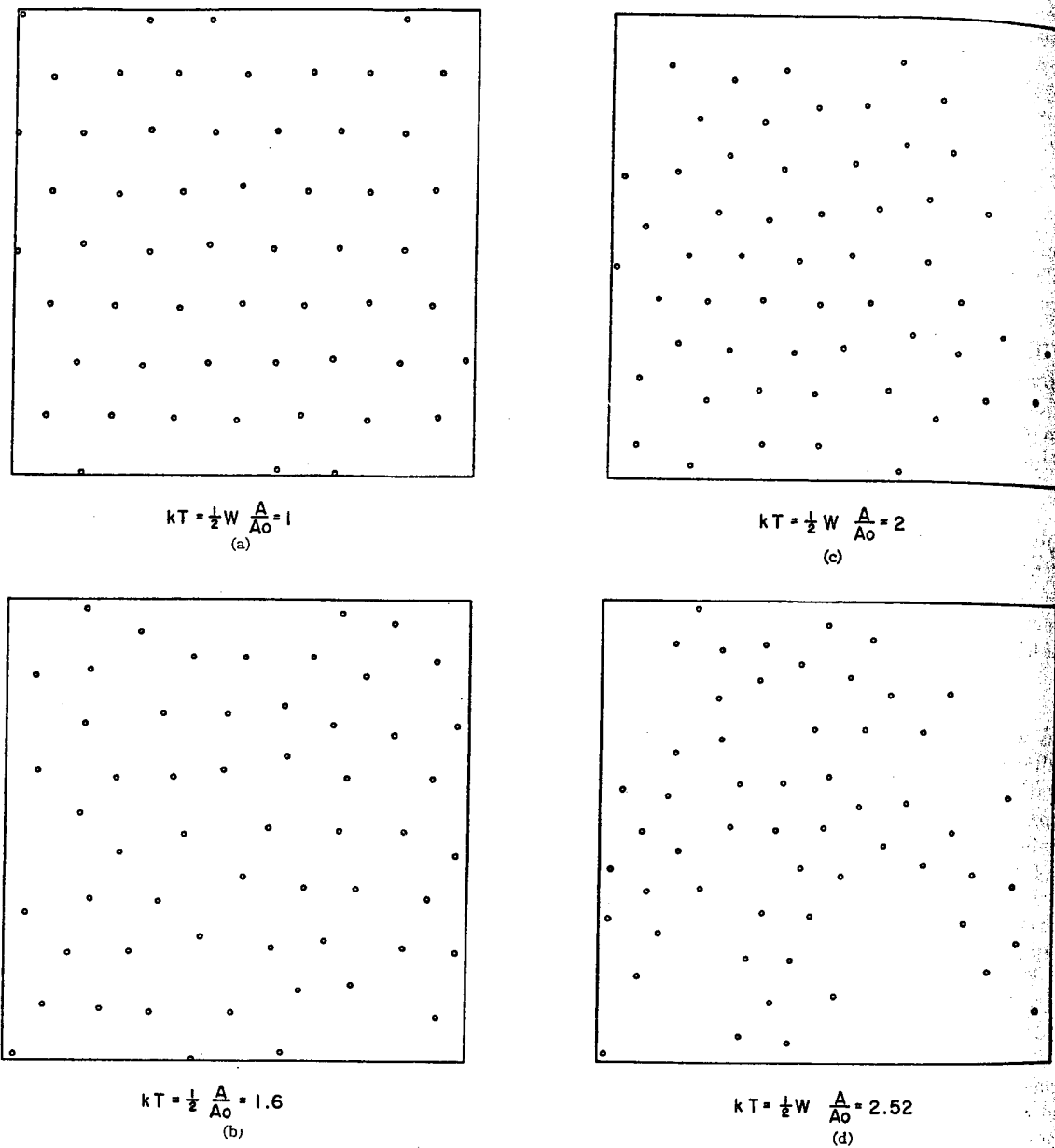


FIG. 4. Typical plots of the positions of the 56 molecules for a two-dimensional system with a Lennard-Jones type interaction between pairs. The temperature is one-half the well depth. The ratio A , the area, to A_0 , the area in a close packed system with the nearest neighbor distance such as to make the potential energy of nearest neighbors zero, is varied from 1 to 2.52 in the four diagrams.

FIG. 4. Lennard Jones Distributions.



Courtesy of the Archives of the Institute for Advanced Study. Photographer: Alan Richards.

John von Neumann, left, with Robert Oppenheimer, Director of the Institute for Advanced Study from 1947-66.

FIG. 5.