Fundamental Problems in
STATISTICAL MECHANICS
A Summer Course

By Gordon Baym

NIJENRODE Castle in Breukelen, the Netherlands, situated between Utrecht and Amsterdam, was home for seventeen days during August of last year to more than sixty physicists, chemists, and advanced students from sixteen countries. These people gathered to attend an intensive course on Fundamental Problems in Statistical Mechanics, held under the auspices of NUFFIC (the Netherlands Universities Foundation for International Cooperation) with support from NATO. Statistical mechanics seemed most appropriately chosen as the subject of the first summer school in theoretical physics in the Netherlands in view of the long tradition, begun by Van der Waals and continued by Ehrenfest, of Dutch research in this field. The lecturers at Nijenrode representing that tradition as it is active in Holland today included N. G. van Kampen, B. R. A. Nijboer, L. van Hove, N. M. Hugenholtz, E. G. D. Cohen, and P. Mazur. Visiting lecturers from abroad were K. Huang of the Massachusetts Institute of Technology, H. Wergeland of the Norwegian Technical High School in Trondheim, and G. E. Uhlenbeck of the Rockefeller Institute in New York.

The course began with a series of review lectures by Nijboer which provided the necessary background for appreciating the more recent developments in the subject. Wergeland, in his lectures, discussed the theory of stochastic processes, which underlies so much of

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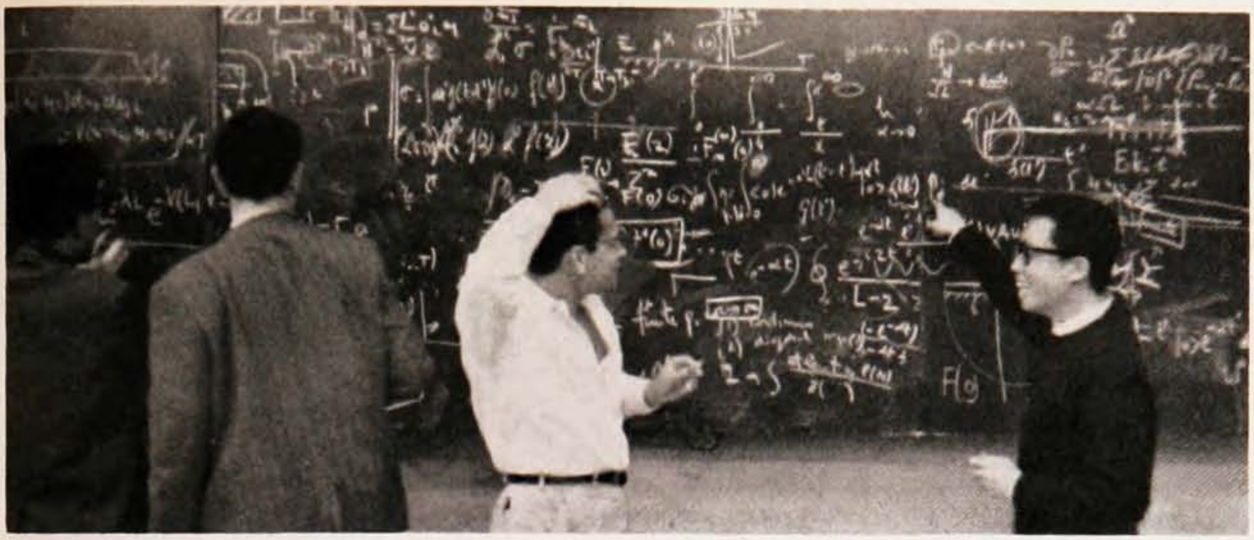


Some of the spirit of the first NUFFIC-sponsored international summer school in theoretical physics in the Netherlands, held in the castle shown on the opposite page, is reflected in these snapshots taken during the 17-day course.

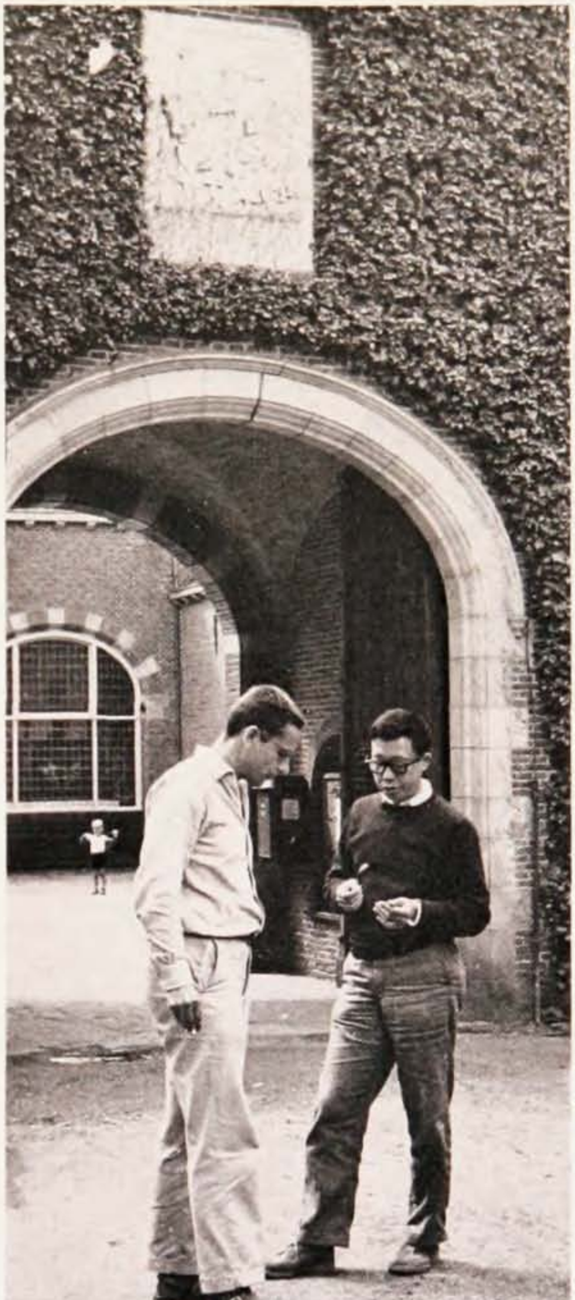
the work in nonequilibrium statistical mechanics. He defined and classified these processes, and gave some of the mathematical tools used in describing them. As particular examples, he treated the theory of fluctuations, the analysis of ionization tracks, and a special model of Brownian motion.

By and large most of the material presented by the lecturers is already in the literature, but there did emerge, as the special contribution of the course, a clear over-all picture of the fundamental problems in statistical mechanics. These can be divided roughly into two classes, equilibrium and nonequilibrium, though the two are by no means unrelated.

Among the important equilibrium problems is that which involves the understanding of phase transitions and, in particular, condensation phenomena and critical points. This problem was the subject matter of lectures by Uhlenbeck, who first reviewed the Yang-Lee theory of condensation, and on this basis was able to show the improbability of being able to predict a condensation starting from the Mayer cluster expansion in the gas region and analytically continuing in the fugacity. He then discussed the work done by Kac and himself on a one-dimensional model of a gas whose atoms have a hard core and an exponentially decaying attractive potential. Solving exactly for the partition function of this model, they found that there is no phase transition as long as the range of the potential is finite. However, they then extended the range to infinity, keeping the product of the depth and range constant. In that limit, it turned out that the gas exhibited a first-order phase transition with a critical point. Furthermore, they showed that the Van der Waals equation, with the Maxwell construction, is the correct equation of state.

Also important among the equilibrium problems is the understanding of interacting quantum-mechanical systems at finite temperature. It has only been in the past six years that a systematic approach to the statistical mechanics of interacting particles has been established. This recent treatment, based on the formalism of the many-body problem, was discussed by Hugenholtz. Considering the fermion problems in detail, he outlined a derivation in perturbation theory of the linked cluster expansion of the logarithm of the partition function. Then he considered the relation of the zero-temperature limit of the finite-temperature perturbation theory to ordinary Brueckner-Goldstone ground-state perturbation theory and the role of the "anomalous" graphs in this limit.

Concerning himself with another aspect of the problem of interacting quantum systems, Huang gave a summary of what can be understood about liquid helium below the lambda point on the basis of the assumption that the low-lying excited states can be described in terms of phonons and rotons in the manner of Feynman and Cohen. Most equilibrium properties, such as second sound, are well understood in this picture. But, Huang emphasized, our understanding of superfluid flow from first principles is still rather poor.



Profs. N. G. van Kampen (Netherlands) and K. Huang (USA) in front of the entrance gate at Nijenrode.

Much of the interest in nonequilibrium statistical mechanics centered on the question of irreversibility and the approach to equilibrium. The program here, as outlined by Uhlenbeck, is that of beginning with the reversible microscopic equations of motion, and, by neglecting correlations, deriving from these some form of irreversible equation, from which one can prove an H- theorem and thereby establish that approach of the system to equilibrium. This equation should also enable one to calculate the various relaxation times of the system and, therefore, the rate of approach to equilibrium. In its most popular form this equation is the "master" equation for the diagonal elements of the density matrix. Passing from such an equation to the phenomenological equations is yet another step, in which one must make use of the conservation laws, e.g., the continuity equation.

Cohen gave a detailed treatment, for a classical gas, of the transition from microscopic equations to macroscopic hydrodynamic equations. The intermediary he used was the Boltzmann equation. His starting point was the Born-Green-Kirkwood hierarchy of coupled equations for the many-particle distribution functions; the hierarchy derived from the Liouville equation. His next step was to outline the Bogoliubov theory for nondilute gases. In this theory, three stages are distinguished. About the initial, or transient stage, one can say nothing. The theory purports to describe the kinetic stage, lasting for times of the order of a mean-free-flight time. The final, or hydrodynamic stage, is the one described by the conservation laws and the familiar phenomenological equations. In the kinetic stage, the many-particle distribution functions, f_2, f_3, etc. at any given time are assumed to be uniquely determined by the one-particle distribution function f_1 at that time. This assumption, together with the assumption that at time minus infinity the particles are uncorrelated, enables one to write down an equation for f_1 in terms of an expansion in the density. To first order this is the familiar Boltzmann equation. Cohen also described the next order term, which involves three-particle correlations. In this way Cohen showed how the transport coefficients might be computed to higher order in the density. However, Van Kampen pointed out that a crucial question of statistical mechanics is the correct choice of the stochastic variables. In particular, he expressed doubt that Bogoliubov's choice of the single-particle distribution function during the kinetic stage is correct.

The nature of the hydrodynamic state was given great attention by Mazur in his lectures on the statistical basis of irreversible thermodynamics. First he set up

a description of the behavior of macroscopic variables in terms of a Markov process, which he then showed could be taken to be Gaussian. From this he derived the Onsager relations and the phenomenological laws for the case that the variables are far from their equilibrium values. Then he showed that in this region both the Gibbs and Boltzmann entropies, defined in terms of the macroscopic variables, increase monotonically, and he explicitly demonstrated that the difference between the two was always negligible.

Van Kampen spoke about the assumptions that have to be added to the microscopic equations of motion for general systems, to arrive at irreversible macroscopic equations. His view is that one must first perform a coarse graining, dividing phase space into cells in each of which the macroscopic variables take on approximately constant values. In quantum mechanics, these phase cells are linear subspaces of Hilbert space. He argued that to define the transition probabilities between these cells a repeated randomness assumption is essential. This assumption leads immediately to the master equation.

Van Hove presented an alternative derivation of the master equation for a quantum system. He also considered a coarse-grained probability density, but differed from Van Kampen in his interpretation of the role of the randomness assumption. In particular he showed how a single randomness assumption on the phases of the states at an initial time was sufficient to derive, in the limit of a weak perturbing interaction, the validity of the master equation for times of the order of the relaxation times. He considered effects of higher orders in the potential and derived an equation for the probability distribution valid to all orders in perturbation theory. This equation did not, however, exhibit Markovian character beyond the lowest order; yet van Hove was able to show for a special example how, to arbitrary order, the approach to equilibrium still occurred.

Supplementing the lectures were several interesting seminars. H. B. G. Casimir spoke about the third law of thermodynamics; J. M. J. van Leeuwen discussed the calculation of pair-distribution functions for gases, and D. ter Haar gave an application of certain Green's-function techniques to an interacting spin system. E. W. Montroll showed a detailed calculation of the recurrence times of a system of independent harmonic oscillators and was able to demonstrate explicitly the connection between the irreversibility and the number of degrees of freedom of the system. Uhlenbeck, in his talk on the statistical mechanics of plasmas, underlined the lack, to date, of a complete derivation of magnetohydrodynamic equations starting from the microkinetic equations.

The lectures and the seminars, between them, provided a very good over-all picture of recent statistical mechanics. Arrangements were made for publication of the proceedings of the course by the North-Holland Publishing Company.