MATHEMATICAL METHODS IN SOLID STATE AND SUPERFLUID THEORY

Scottish Universities' Summer School
1967

Edited by
R. C. CLARK, B.A., PH.D.
and
G. H. DERRICK, B.SC., PH.D.

OLIVER & BOYD
EDINBURGH

OLIVER AND BOYD LTD

Tweeddale Court

Edinburgh 1

FIRST PUBLISHED 1969

05 001 67 7 6 handbook
05 001 67 8 4 paperback

Printed in Great Britain by
Robert Cunningham and Sons Ltd
Alva, Scotland

PREFACE

THE 8th Scottish Universities' Summer School in Physics was held in St Andrews from 31st July to 19th August 1967, the chosen field being "Mathematical Methods in Solid State and Superfluid Theory". Generous financial support from the NATO Scientific Affairs Division and from all eight Scottish Universities helped us to assemble an exceptionally distinguished panel of lecturers, and to award a number of bursaries to highly qualified students wishing to come from distant countries.

Originally the intention had been to offer a course in mathematical methods at early postgraduate level for theoreticians, or correspondingly late postgraduate level for experimentalists. However, at a very early stage of planning it was discovered that the organizers of the Les Houches Summer Schools had simultaneously developed much the same plan for just the same summer vacation. It was thereupon agreed that Les Houches would provide a course on many-body theory primarily for experimental physicists, while St Andrews would cater specifically for theoretical physicists of at least one year's postgraduate standing. In all, three hundred applications were received for the seventy student places available at the School. Our thanks are due to the members of the Selection Committee for carrying through their onerous and unenviable task expeditiously and efficiently.

As indicated by the title, the general plan of the Summer School was to develop those mathematical methods which are proving most valuable in current research in solid state and superfluid theory. It was accepted from the start that in a School extending only over three weeks important areas of development would simply have to be omitted: in particular, topics as yet primarily of mathematical rather than physical interest, and even any attempt at systematic group theory—though the ideas of the group theoretical approach are naturally inherent in some of the lectures, for instance those on transformation theory. The eight main lecture courses, which all students were expected to attend, were supplemented by a series of advanced seminars in which recent research was reported and discussed by the experts in the field. One such seminar was notably up to date, being largely devoted to research carried out during the period of the School!

Finally, as Director I would like to express my thanks to all those who contributed to the success of this School: above all, to our ever-efficient Secretary Dr C. G. Kuper, quite undeterred by having at the same time to make final preparations for his move to Haifa; to our Steward, Arne Børs, whose organizing capacity, vigilance and hard work proved so valuable in Hamilton Hall where the great majority of participants were accommodated;

to Dr W. M. Young, our Treasurer, and to other members of the Executive Committee and their wives; and to the University Court for holding an official Dinner in association with the School. This collected record of the scientific proceedings is itself sufficiently indicative of our debt to the joint Editors, Dr R. C. Clark and Dr G. H. Derrick.

R. B. DINGLE
Professor of Theoretical Physics,
University of St Andrews

EDITORS' NOTE

WITH the exception of chapters 6 and 8 these proceedings are based on manuscripts provided by the authors and revised by them to incorporate points raised in the discussions which followed the lectures. Chapter 6 is limited to a synopsis and bibliography, the lecturer holding the view that equivalent material on this topic is already easily accessible in the literature. The manuscript for chapter 8 was prepared by our note-takers and revised by the lecturer.

We wish to thank Mrs C. G. MacArthur, Mr T. McQueen and Mr D. L. T. Anderson for their skilled clerical, technical and draughting assistance in preparing the preprints and final typescripts, and also the many official note-takers who devoted a considerable amount of their time to preparing clear records of the lectures.

R. C. CLARK
G. H. DERRICK

EXECUTIVE COMMITTEE OF THE 1967 SUMMER SCHOOL

Professor R. B. Dingle,	St Andrews,	*Director.*
Dr W. M. Young,	Dundee,	*Treasurer.*
Dr C. G. Kuper,*	St Andrews,	*Secretary.*
Mr A. Børs,	St Andrews,	*Steward.*
Dr R. C. Clark,†	St Andrews,	*Joint Editor.*
Dr G. H. Derrick,	St Andrews,	*Joint Editor.*
Mr N. C. McGill,	St Andrews.	
Dr E. W. Laing,	Glasgow.	

* Now professor at the Technion, Haifa.
† Now at University of California, San Diego, La Jolla.

LECTURERS

Courses

Professor G. Baym, Illinois
Professor K. A. Brueckner, University of California, San Diego
Dr C. De Dominicis, Saclay
Professor E. P. Gross, Brandeis
Professor C. Lanczos, Dublin
Professor E. H. Lieb, Northeastern
Professor J. M. Luttinger, Columbia
Professor J. G. Valatin, Queen Mary College, London

Seminars

Dr D. J. Amit, Cornell
Professor C. P. Enz, Geneva
Dr A. Huber, Birmingham
Dr Y. Imry, Soreq Nuclear Research Centre, Israel
Professor R. V. Lange, Brandeis
Professor N. March, Sheffield
Dr E. Riedel, Max-Planck Institut, Munich

PARTICIPANTS

Mr M. R. Aish, Oxford
Dr D. Amit, Cornell, *guest*
*Mr J. Armitage, St Andrews
Mr A. Aviran, Technion, Haifa

Mr J. F. Balsley, Indiana
Professor J. Bardeen, Illinois, *guest*
Mr A. J. F. Bastin, Ecole Normale Supérieure, Paris
Professor G. Baym, Illinois
Dr D. E. Beck, St Andrews, *observer*
Mr G. G. Bjorkman, Göteborg
Mr E. Bonderup, Aarhus
Mr P. Borckmans, Université Libre de Bruxelles
Mr A. Børs, St Andrews
Dr Elizabeth Bradford, Harwell
Mr P. Brand, Stuttgart
*Dr M. G. Brereton, Leeds
*Mr A. M. Brett, St Andrews
Professor K. A. Brueckner, University of California, San Diego
Mr R. J. Buchler, University of California, San Diego

Dr R. C. Clark, St Andrews
Mr M. G. Cottam, Oxford

Mr A. E. Davis, Newcastle-upon-Tyne
Dr G. H. Derrick, St Andrews
Miss Karin Dichtel, Kiel
Professor R. B. Dingle, St Andrews
Mr L. Dobrzynski, Lille
Dr C. De Dominicis, Saclay

Mr H. A. M. van Eekeelen, Nottingham
Professor C. P. Enz, Geneva, *observer*
*Mr A. G. Every, Reading

Dr D. M. Finlayson, St Andrews, *observer*
Mr J. R. Fletcher, Nottingham
Mr L. J. Fletcher, Imperial College, London
Dr I. Giaever, General Electric, Schenectady, *observer*
Mr N. G. Grimvall, Göteborg
Professor E. P. Gross, Brandeis
Dr L. Gunther, Orsay
Dr B. L. Gyorffy, Queen Mary College, London

Mr D. C. Herbert, Imperial College, London
Mrs Rosemary Herbert, Westfield College, London
Dr A. Huber, Birmingham, *observer*
Mr R. A. Hunt, Queen Mary College, London
*Mr G. J. Hyland, Liverpool

Dr Y. Imry, Soreq Nuclear Research Centre, Israel

Dr H. F. G. Keiter, Göttingen
Mr P. H. Kleban, Brandeis
Mr R. H. Knapp, Jr., Oxford
Mr K. Kral, Prague
Professor O. Krisement, Münster, *observer*
Mr N. J. Kupelian, Brandeis
Dr C. G. Kuper, St Andrews

Dr E. W. Laing, Glasgow
Professor C. Lanczos, Dublin
Professor R. V. Lange, Brandeis, *guest*
*Dr P. L. Leath, Oxford
*Dr J. Lekner, Université Libre de Bruxelles
Professor E. H. Lieb, Northeastern
Mr B. W. Lix, Stuttgart
*Mr R. J. Loader, Reading
Professor J. M. Luttinger, Columbia

Professor C. McCombie, Reading, *guest*
Dr N. MacDonald, Glasgow, *observer*
Mr N. C. McGill, St Andrews
Professor N. March, Sheffield, *guest*
Dr W. Moorman, Göttingen
Mr G. Morandi, Bologna
Mr M. J. Morris, Leeds
Mr J. P. Muller, Geneva

Mr M. J. O'Connor, Queen Mary College, London

Mr R. Pirc, Ljubljana
Miss G. Pizzichini, Bologna
*Mr C. M. Place, Leeds

Mr J. Rae, Glasgow
Dr C. F. Ratto, Genova
*Mrs Martha H. Redi, Rutgers
Professor H. G. Reik, Freiburg, *observer*

*Official note-takers

Mr J. F. Renardy, Saclay
Dr E. Riedel, Max-Planck Institut, Munich
Mr P. Rijnierse, St Andrews

Mr W. F. Saam, Illinois
Mr J. Sak, Prague
Mr J. Slechta, Prague
Dr J. A. Snow, Washington University, St Louis

Mr K. Timmesfeld, Frankfurt
Mr G. Toulouse, Orsay

Professor J. G. Valatin, Queen Mary College, London
Dr P. Vashishta, St Andrews
Mr G. Vertogen, Groningen

Mr L. Warsztacki, Université Libre de Bruxelles
Mr D. L. Weaire, Cambridge
Mr W. Wonneberger, Freiburg

Dr W. M. Young, Dundee
Mr G. Yuval, Cambridge

CONTENTS

14. VARIATIONAL PRINCIPLES IN QUANTUM STATISTICAL MECHANICS

ALBRECHT HUBER

15. RIGOROUS LOWER BOUNDS ON PARAMAGNETIC SUSCEPTIBILITY

ROBERT V. LANGE

1

VARIATIONAL PRINCIPLES

C. LANCZOS
Institute for Advanced Studies, Dublin

1

HISTORICAL SURVEY

1.1. *Introduction*

THE search for the ultimate principles of the physical universe was a popular field of contemplation throughout the ages. Even up to our own time we made no great progress in the question, whether we will forever stay on the surface of things and never come to grips with the "great ocean of truth", as Newton called it, or gradually approach something that we could consider as basic to all physical phenomena. More often than not the human mind tried to read something into the workings of nature, as if nature attempted to achieve something, as if nature were imbued with a mathematical intelligence. Although the idea is of a metaphysical character and in apparent contradiction to the causal way of thinking, yet in all periods of history the concept had its fascination. The earliest example is undoubtedly the straight line as the shortest communication between two points. But Hero of Alexandria (first century A.D.) observed already that the laws of optical reflection could be obtained from the principle that light starting at A and reaching B via the mirror at C should reach its destination in the shortest possible time. Later, when the law of optical refraction was discovered, this law was again in full harmony with the same principle, which Fermat raised to a universal principle of optics. Hence all the phenomena of geometrical optics could be derived from the single principle that light proceeds along such a path, which will make the time of travel between the point of departure and the point of arrival a minimum. In the application of this principle the assumption is made that the velocity of light propagation is a given quantity at every point of the optical path.

Later in the analysis of mechanical phenomena a similar development took place. Influenced by certain teleological ideas of Leibniz, the philosophers of the eighteenth century investigated the possibility that perhaps the laws of mechanical action, discovered by Newton, are the consequences of an all-embracing minimum principle. Here again their efforts were crowned with success. From a somewhat obscure and incomplete formulation of Maupertuis, the great analysts Euler and Lagrange arrived at a principle, called "principle of least action", which permitted to conceive all mechanical action as the consequence of minimizing a certain quantity associated with the mechanical motion, and defined as "action". Once more the idea was victorious that there is a tendency in nature to reduce a certain quantity, that one could consider as the measure of mechanical action, to a minimum. Lagrange developed an entirely new branch of mathematics, called the "calculus of variations", to cope with this type of problems. In his *Méchanique Analytique* (1788) he realized the tremendous possibilities of the new discipline, not so much for its philosophical and metaphysical implications, as for the great perspectives which opened up to the enquiring mind. The Newtonian form of mechanics was individualistic, every particle moving according to the more or less accidental force which acted on it. Lagrange's mechanics was universalistic. The individual particle meant nothing, the mechanical *system* came in the foreground. The system acted as a whole, and a single function, the "Lagrangian function L", dominated the entire phenomenon. If this function was given and we knew the initial parameters of the system, the rest was mere mathematical computation. This feature of the Lagrangian method raised it far beyond the limitations of Newtonian mechanics. A single scalar function was the unifying link in an infinite variety of apparently disconnected motion phenomena. Moreover, whereas Newton's mechanics was strongly linked to the Cartesian type of coordinates, the Lagrangian function could be given in arbitrary curvilinear coordinates and thus displayed a flexibility, which was of greatest importance in the solution of involved mechanical problems.

In the beginning of the nineteenth century the emphasis shifted to the idea of a *field*, instead of the motion of discrete particles. The ideas of Fresnel and Faraday became of dominant importance, and Maxwell succeeded in a mathematical formulation of Faraday's physical ideas, which comprised in the form of eight partial differential equations, the celebrated "Maxwellian equations", a tremendous variety of optical and electromagnetic phenomena. Although the efforts to reduce these equations to the mechanical motion of particles were not successful and the attempt to reduce all physical phenomena to hidden motions was eventually abandoned, yet the principle of least action was once more triumphant. Once more the fundamental Lagrangian could be found, from which the Maxwellian equations were obtainable by the process of variation.

The later development of physics was not less influenced by variational methods. Newtonian mechanics gave way to relativistic mechanics. Euclidean geometry was replaced by Riemannian geometry. The field equations of classical physics were completely revised by quantum theory and many cherished ideas of the past had to be abandoned. Yet it is astonishing to see that through all these changes one thing remained unchanged, viz. the possibility of submitting all our equations to the operation of a variational principle. Relativistic mechanics re-interpreted the kinetic energy of Newtonian physics on the basis of the four-dimensional line element, but the existence of a Lagrangian was not challenged. Only the form of the Lagrangian changed. The field equations of Einstein's gravitational theory were deducible from a basic Lagrangian, the scalar curvature. Schrödinger's wave equation possessed a Lagrangian and in fact the most important feature of wave mechanical equations is their self-adjoint character, which is equivalent to the existence of a variational principle. The same holds of most of the equations of quantum field theory.

Let us discuss in somewhat more detail the fundamental aspects of the variational method. The most striking feature of the procedure is that in spite of the apparently purpose-oriented nature of the principle it is in full harmony with the causal way of thinking. Along the minimum path from A to B let us pick out a point C, which can be as near to A as we wish. If the path AC would not be a minimum path in itself, a better local minimum would improve also on the total minimum. Hence any part of a minimum path is in itself a minimum path. We can string together any number of minimum paths, observing certain conditions of continuity at the end points, and obtain thus the resulting path in the large, by putting together a large number of local minimum paths. The original problem may involve two points which are very far from each other. But to obtain the path from A to the nearer point C does not demand any knowledge of what happens beyond C, provided that we have started from A in the right direction.

The earliest application of a minimum principle to a physical phenomenon is reportedly the method of Heron of Alexandria, who derived the law of optical reflection by a minimum principle. The problem of minimizing the time of propagation can be solved by simple algebra and yields the condition that the angle of incidence and the angle of reflection must be equal. Later, when the law of optical refraction was experimentally established, the same principle demonstrated its value again. Consider two media, the medium I in which light propagates with the velocity v_1 and the medium II, in which light travels with the velocity v_2 (see Fig. 1). Then the problem of minimizing the time of travel between A and B demands that we should find the position of the point Q by the condition that

$$t_1 + t_2 = s_1/v_1 + s_2/v_2$$

shall become a minimum. The solution of our problem is that the point Q must be chosen according to the condition

$$(\sin \alpha)/v_1 = (\sin \beta)/v_2$$

which agrees with the observed law of refraction.

The remarkable analogy between optical and mechanical phenomena