

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

© 1969, The Authors

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

PREFACE

HE 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;

vi

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

TITH 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.

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

[†] Now at University of California, San Diego, La Jolla.

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,

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

San Diego

London

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
Mrs Rosemary Herbert, Westfield College,
London
Dr A. Huber, Birmingham, observer

Mr D. C. Herbert, Imperial College,

Mr R. A. Hunt, Queen Mary College,

*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

	PAGE
PREFACE by Professor R. B. DINGLE	v
EDITORS' NOTE	vi
Executive Committee of the 1967 Summer School	vii
Lecturers	vii
Participants	viii
1 WARIATIONAL PRINCIPLES	C I WCZOS
1. VARIATIONAL PRINCIPLES	C. LANCZOS
1. Historical Survey	1
1.1. Introduction	1
1.2. The Lagrangian equations of motion	8
1.3. The method of the Lagrangian multiplier	9
1.4. Elimination of algebraic variables	9
1.5. Elimination of kinosthenic variables	9
1.6. Hamilton's canonical equations	10
1.7. Canonical transformations	11
1.8. The partial differential equation of Hamilton-Jacobi	11
1.9. Infinitesimal canonical transformations	13
1.10. The Lagrange and Poisson brackets	14
2. Partial Operators	15
2.1. The mechanics of continua	15
2.2. The Hamiltonization of partial operators	16
2.3. Hamiltonian form for Lagrangians containing higher derivati	
the first	18
2.4. Orthogonal function systems	21
2.5. Direct minimization methods	28
3. Noether's Theorem and the Conservation Laws	30
3.1. Introduction	30
3.2. The conservation of momentum	31
3.3. The conservation of angular momentum	33
3.4. The conservation of energy	34
3.5. The conservation laws of field physics	34
3.6. The Maxwellian equations	36
3.7. The Schrödinger equation	37
3.8. The Dirac equation	38
3.9. Coordinate transformations	38
3.10. The symmetric energy-momentum tensor	41
3.11. The ten conservation laws and the motion law of a particle	43
2. TRANSFORMATION THEORY EUGE	NE P. GROSS
1. Introduction and Elementary Examples of Canonical Transformation	ns 46
1.1. Introduction	46

xii CONTENTS

	PAGE
1.2. Scale change for the Bose oscillator	49
1.3. One-dimensional moving wall problem	51
1.4. Displaced oscillator	52
1.5. The Bogolyubov transformation as a scale transformation 1.6. General remarks	55 58
1.6. General remarks	36
2. Adiabatic Switching Techniques	59
2.1. Analysis of the transformation function	59
2.2. Adiabatic switching and the forced harmonic oscillator	63
2.3. Proof of the adiabatic theorem and level-shift formulae	67
3. Perturbation Formulae	69
3.1. Exponential form for U	69
3.2. Evolution operator in energy space	72
4. Non-Relativistic Particle-Field Problem	79
4.1. Introduction	79
4.2. Preliminary kinematical consideration	80
4.3. Correlation functions	82
4.4. Green's functions for the no-recoil case	84
4.5. Heisenberg operator equations for the no-recoil case	87
4.6. Classical analysis with field description of sources	89
5. Analytic Approaches to the Particle-Field Problem	95
5.1. Manifestly translation invariant methods	95
5.2. Non-translationally invariant theories	104
5.3. Strong coupling with field description of source	106
6. Point Transformations	109
6.1. Introduction	109
6.2. The one-body problem	110
6.3. The many-body problem	114
6.4. Point transforms	118
3. THE MICROSCOPIC DESCRIPTION OF SUPERFLUIDITY	
46	GORDON BAYM
1. Introduction	121
2. Condensates	122
. Statistical Mechanics of Moving Systems	129
4. Normal Mass Density and Moment of Inertia of a Superfluid	134
5. Linear Response Theory	143
6. Why is $\rho_n < \rho$ in a Superfluid?	149
7. A Relation between ρ_s , $ \Psi ^2$ and the Fluctuations of the Conder	nsate 151

CONTENTS	xiii
TRANSPORT THEORY	J. M. LUTTINGER
	PAGE
 Phenomenological Description 1.1. A note on the use of the phenomenological equations 	157 162
2. General Theory of the Transport Coefficients	163
3. Independent Electrons	170
4. Transport Equation	173
5. Derivation of the Transport Equation	177
DENSITY MATRIX METHODS AND SUPERCONDUCTIVE	VITY THEORY J. G. VALATIN
1. Introduction	194
2. Density Matrix Form of the Hartree-Fock Equations	195
3. Elements of Superconductivity Theory	201
4. Matrix Equations, Current Response	207
5. Competitive Coupling Effects	214
6. Quasi-Particles at Thermal Equilibrium	219
7. Superconducting Films in a Magnetic Field	224
QUANTUM STATISTICAL MECHANICS BY PERTURBATE RESUMMATION METHODS	ΓΙΟΝ C. DE DOMINICIS
Synopsis and Bibliography	233
1. Perturbation Theory of Normal Systems	233
2. Linear Responses	233
3. Superfluid Systems by Perturbation Resummation Methods	234
PERTURBATION THEORY AND ITS APPLICATIONS	K. A. BRUECKNER

4.

5.

6.

7.

1.1. Introduction

1.2. The uniform electron gas

1.4. Application to atoms

1.3. The non-uniform electron gas

235

235

235

240

251

1. The Correlation Energy of Electrons in Non-Uniform Systems

CONTENTS

 The Charged Boson Gas 1. Introduction Ring diagrams Application of field-theoretic methods General features of the excitation spectrum Applications 	252 252 255 260 268 269
 3. Solid He³ 3.1. Introduction 3.2. Short-range correlations 3.3. Long-range correlations 	275 275 276 281
8. EXACTLY SOLUBLE MODELS	ELLIOTT H. LIEB
1. Heisenberg Chain	286
2. Two-Dimensional Ising Model	291
3. Heisenberg Chain (continued)	294
4. Ice Model	297
5. KDP and F Models	304
 9. EFFECTIVE LONG-RANGE ORDER AND PHASE TRAN ONE-DIMENSIONAL SYSTEMS 10. PARTICLE-HOLE EXCITATIONS AND SELF ENERGY 	Y. IMRY 307 OF QUASI-
PARTICLES IN A FERMI LIQUID	DANIEL J. AMIT
1. Introduction	312
2. Recapitulation	313
3. Properties of the Vertex Function	314
4. Landau Limits	315
5. Equations for the Mass Operator	316
 Behaviour of the Mass Operator near the Fermi Surface and the Logarithmic Terms 	ne Origin of the
7. The Inconsistency and its Resolution	320
8. The Correction to the Damping	321
9. Quasi-Particle Energy	321

CONTENTS	×۷
 10. The Specific Heat of a Fermi Liquid 10.1. Introduction 10.2. Recapitulation and definitions 10.3. Expansion of Y to first order in G' and M' 10.4. Expansion in terms of δf 10.5. The entropy and the specific heat 10.6. The second-order terms in the temperature expansion 10.7. Conclusion 	9AGE 322 322 322 323 324 326 328 330
11. RENORMALIZED THEORY OF LOW TEMPERATURE SPECIFIC HEAT OF LIQUID He ³ EBERHARD	RIEDEL
1. Introduction	332
2. Functional Representation of the Thermodynamical Potential	333
3. The Thermodynamical Potential $Y[G]$ in SPA	334
4. Low-Temperature Expansion of $Y[G]$	336
12. PHONON-PHONON INTERACTION AND SECOND SOUND IN DIELECTRICS CHARLES P. ENZ	339
13. ASYMPTOTIC BEHAVIOUR OF CORRELATION FUNCTIONS IN CLASSICAL AND QUANTAL FLUIDS $N.\ H.$	MARCH
1. Introduction	348
 Forces and Particle Correlations in Classical Fluids Ornstein-Zernike direct correlation function Asymptotic forms of h(r) and c(r) for van der Waals fluids Asymptotic forms for point-ion model of liquid metal Exponentially decaying interactions 	349 350 351 353 354
 3. Quantal Fluids 3.1. Liquid ⁴He at T = 0 3.2. Hard-sphere bosons 3.3. Non-interacting fermions 3.4. Interacting electron gas 3.5. Some inferences on liquid ³He 	354 354 356 356 357 358
 4. Dynamics and Time-dependent Behaviour of Correlation Functions 4.1. Van der Waals classical fluids 4.2. Liquid ⁴He 4.3. Non-interacting fermions 	359 359 360 360
5. Conclusion	362

xvi CONTENTS

14. VARIATIONAL PRINCIPLES IN QUANTUM STATISTICAL MECHANICS ${\it ALBRECHT~HUBER}$

	PAGE
1. Introduction	364
2. General Extremum Principle for Thermodynamic Potentials	367
3. Relation of Feynman's Variational Principle to Bogolyubov's Theorem	373
4. Stability Criterion for the Thermal Hartree-Fock Approximation	377
 Unitary Transformations to Quasi-Particle Coordinates in the Variational Method 	382
 The Case of Linear Relations between Bare Particle and Quasi-Particle Co- ordinates 	385
7. Approximations for Unitary Transformations	389
15. RIGOROUS LOWER BOUNDS ON PARAMAGNETIC SUSCEPTIBILIT ROBERT V. L	
1. Introduction	393
2. Definition of the Problem	393
3. The Fundamental Inequality	395
4. The Choice of Operator C_k^{\dagger}	396
5. Variational Treatment of C_k^{\dagger}	397
6. "Best Bound" for the Free Gas	399
7. Conclusions and Prospects	400

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

MMSS B

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