

# 7 Springer Series in Solid-State Sciences

Edited by Peter Fulde

---



# Springer Series in Solid-State Sciences

Editors: M. Cardona P. Fulde H.-J. Queisser

---

- Volume 1 **Principles of Magnetic Resonance** 2nd Edition  
By C. P. Slichter
- Volume 2 **Introduction to Solid-State Theory**  
By O. Madelung
- Volume 3 **Dynamical Scattering of X-Rays in Crystals**  
By Z. G. Pinsker
- Volume 4 **Inelastic Electron Tunneling Spectroscopy**  
Editor: T. Wolfram
- Volume 5 **Fundamentals of Crystal Growth I. Macroscopic Equilibrium  
and Transport Concepts**  
By F. Rosenberger
- Volume 6 **Magnetic Flux Structures in Superconductors**  
By R. P. Huebener
- Volume 7 **Green's Functions in Quantum Physics**  
By E. N. Economou
- Volume 8 **Solitons and Condensed Matter Physics**  
Editors: A. R. Bishop and T. Schneider
- Volume 9 **Photoferroelectrics**  
By V. M. Fridkin
- Volume 10 **Phonon Dispersion Relations in Insulators**  
By H. Bilz and W. Kress

E. N. Economou

# Green's Functions in Quantum Physics

With 49 Figures

Springer-Verlag Berlin Heidelberg GmbH 1979

Professor Eleftherios N. Economou, PhD

Department of Physics, University of Virginia  
Charlottesville, VA 22901, USA

*Series Editors:*

Professor Dr. Manuel Cardona

Professor Dr. Peter Fulde

Professor Dr. Hans-Joachim Queisser

Max-Planck-Institut für Festkörperforschung  
Büsener Strasse 171, D-7000 Stuttgart 80, Fed. Rep. of Germany

ISBN 978-3-662-11902-0 ISBN 978-3-662-11900-6 (eBook)

DOI 10.1007/978-3-662-11900-6

Softcover reprint of the hardcover 1st edition 1979

Library of Congress Cataloging in Publication Data. Economou, E. N., 1940—. Green's functions in quantum physics. (Springer series in solid-state sciences; v. 7). Bibliography: p. Includes index. 1. Green's functions. 2. Quantum theory. I. Title. II. Series. QC174.17.G68E25 530.1'2 78-21304

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically those of translation, reprinting, reuse of illustrations, broadcasting, reproduction by photocopying machine or similar means, and storage in data banks. Under § 54 of the German Copyright Law, where copies are made for other than private use, a fee is payable to the publisher, the amount of the fee to be determined by agreement with the publisher.

© Springer-Verlag Berlin Heidelberg 1979

Originally published by Springer-Verlag Berlin Heidelberg New York in 1979.

The use of registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

Offset printing: Zehnersche Buchdruckerei, Speyer. Bookbinding: J. Schäffer oHG, Grünstadt.  
2153/3130-543210

# Preface

This text grew out of a series of lectures addressed to solid-state experimentalists and graduate students beginning their research career in solid-state physics.

The first part consisting of Chaps.1 and 2 is a rather extensive mathematical introduction which covers the material about Green's functions usually included in a graduate course on mathematical physics. Emphasis is given to those topics which are of significance in quantum physics. On the other hand, little attention is given to the important question of determining the Green's functions associated with boundary conditions on surfaces at finite distance from the source.

The second and main part of the book is, in my opinion, a first effort to collect in a systematic but concise way various topics of quantum physics, where the Green's functions (as defined in Part I) can be successfully applied. Chapter 3 is a direct application of the formalism developed in Part I. In Chap.4 the perturbation theory for Green's functions is presented and applied to scattering and to the question of formation of bound states. Next the Green's functions for the so-called Tight Binding Hamiltonian (TBH) are calculated. The TBH is of central importance for solid-state physics because it is the simplest example of wave propagation in periodic structures. It is also important for quantum physics in general, because it is rich in physical phenomena (e.g., negative effective mass, creation of a bound state by a repulsive perturbation) and, at the same time, simple in its mathematical treatment. Thus one can derive *simple, exact* expressions for scattering cross sections and for bound and resonance levels. The multiple scattering formalism is presented within the framework of the TBH, and it is applied to questions related with the behavior of disordered systems (such as amorphous semiconductors). The material of Part II is of interest not only to solid-state physicists but to students of a graduate course in quantum mechanics (or scattering theory) as well.

In Part III, with the help of the second quantization formalism, the many-body Green's functions are introduced and utilized in extracting phy-

sical information about interacting many particle systems. Many excellent books have been devoted to the material of Part III (e.g., FETTER and WALECKA: *Quantum Theory of Many-Particle Systems* [4.1]). Thus the present-treatment must be viewed as a brief introduction to the subject; this introduction may help the solid-state theorist approach the existing thorough treatments of the subject and the solid-state experimentalist to be acquainted with the formalism.

At the beginning of each chapter, there is a brief summary of what the reader will find in the particular chapter. The summary contains also the most important equations numbered as in the main text of the chapter.

I would like to thank Nuclear Research Center "Demokritos" and the Greek Atomic Energy Commission for their hospitality during the writing of the second half of this book.

November 1978

E.N. Economou

# Contents

## Part I: Green's Functions in Mathematical Physics

1. Time-Independent Green's Functions .....	3
1.1 Formalism .....	6
1.2 Examples .....	13
1.2.1 Three-Dimensional Case .....	13
1.2.2 Two-Dimensional Case .....	15
1.2.3 One-Dimensional Case .....	17
1.2.4 Finite Domain $\Omega$ .....	17
2. Time-Dependent Green's Functions .....	19
2.1 First-Order Case .....	23
2.2 Examples .....	26
2.3 Second-Order Case .....	28
2.4 Examples .....	32

## Part II: Green's Functions in One-Body Quantum Problems

3. Physical Significance of $G$ . Application to the Free Particle Case ..	39
3.1 General Relations .....	41
3.2 The Free Particle ( $H_0 = p^2/2m$ ) Case .....	44
3.3 The Free Particle Klein-Gordon Case .....	47
4. Green's Functions and Perturbation Theory .....	50
4.1 Formalism .....	53
4.1.1 Time-Independent Case .....	53
4.1.2 Time-Dependent Case .....	58
4.2 Application: Scattering Theory ( $E > 0$ ) .....	63
4.3 Application: Bound State in Shallow Potential Wells ( $E < 0$ ) ..	67
5. Green's Functions for Tight Binding Hamiltonians .....	71
5.1 Introductory Remarks .....	72
5.2 The Tight Binding Hamiltonian (TBH) .....	74

5.3	Green's Functions .....	78
5.3.1	One-Dimensional Lattice .....	80
5.3.2	Square Lattice .....	82
5.3.3	Simple Cubic Lattice .....	85
5.4	Green's Functions for Bethe Lattices (Cayley Trees) .....	89
6.	Single Impurity Scattering .....	92
6.1	Formalism .....	94
6.2	Explicit Results .....	102
6.2.1	Three-Dimensional Case .....	102
6.2.2	Two-Dimensional Case .....	105
6.2.3	One-Dimensional Case .....	108
6.3	Applications .....	110
6.3.1	Levels in the Gap .....	110
6.3.2	The Cooper Pair .....	110
6.3.3	Lattice Vibrations in Crystals Containing "Isotope" Impurities .....	112
7.	Two or More Impurities; Disordered Systems .....	116
7.1	Two Impurities .....	116
7.2	Infinite Number of Impurities .....	126
7.2.1	Virtual Crystal Approximation (VCA) .....	127
7.2.2	Average t-Matrix Approximation (ATA) .....	128
7.2.3	Coherent Potential Approximation (CPA) .....	130
7.3	Nature of Eigenstates in Disordered Systems .....	136

Part III: Green's Functions in Many-Body Systems

8.	Definitions .....	145
8.1	Single Particle Green's Functions in Terms of Field Operators .....	146
8.2	Green's Functions for Interacting Particles .....	151
8.3	Green's Functions for Noninteracting Particles .....	156
9.	Properties and Use of the Green's Functions .....	160
9.1	Analytical Properties of the $g$ 's and $\tilde{g}$ 's .....	162
9.2	Physical Significance and Use of the $g$ 's and $\tilde{g}$ 's .....	168
9.3	Quasi-Particles .....	176
10.	Computational Methods for $g$ .....	184
10.1	Equation of Motion Method .....	185
10.2	Diagrammatic Method for Fermions at $T = 0$ .....	190
10.3	Diagrammatic Method for $T \neq 0$ .....	200
10.4	Partial Summations. Dyson's Equation .....	203



11. Applications .....	210
11.1 Normal Fermi Systems. Landau Theory .....	211
11.2 High Density Electron Gas .....	216
11.3 Dilute Fermi Gas .....	224
Appendix A: Analytic Behavior of $G(z)$ Near a Band Edge .....	227
Appendix B: The Renormalized Perturbation Expansion (RPE) .....	230
Appendix C: Second Quantization .....	235
<i>References</i> .....	245
<i>Subject Index</i> .....	249