GREEN FUNCTIONS FOR ORDERED AND DISORDERED SYSTEMS

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To my mother

and to my family

Preface

This book is an attempt to satisfy the need for a relatively self-contained exposition of the use of Green functions and multiple-scattering theory in the study of the electronic structure of matter, at a low enough level of sophistication to be accessible to graduate students embarking on their research career. Although one can find a number of books or monographs in which Green functions and their application to the study of condensed matter physics are adequately presented, there appears to be no similar exposition of multiple scattering theory, particularly directed to students.

A number of other formal approaches to the calculation of electronic structure have found expression in essentially text book form, with these of augmented plane waves and of linear muffin-tin orbitals being notable examples. From personal experience and from conversations with colleagues, the lack of a comparable exposition of Green functions based on multiple-scattering theory emerged as particularly prominent. Further, given the great formal and computation power emanating from a combination of these two constructs, Green functions and multiple scattering theory, it appeared of essence to acquaint those beginning their research in the field of electronic structure with this elegant and versatile computation tool.

When originally conceived, this book was to contain only an exposition of the use of Green functions in the study of substitutionally disordered materials, particularly within the coherent potential approximation (CPA). However, it quickly became apparent that a project of such a narrow scope would hardly be self-contained, let alone provide an adequate introduction to its subject for the beginner. Consequently the book grew, both in breath and in depth. In its final form, it is divided into two parts. The first contains a rather informal discussion of Green functions and multiple scattering theory within the tight-binding approximation to the Hamiltonian of a solid, and their application to the study of substitutionally disordered alloys. Several attempts at a cluster generalization or extension of the CPA are also discussed there. The second half presents a somewhat more rigorous exposition of Green functions and multiple scattering theory within a first-principles formalism, and their application to the calculation of the electronic structure of pure, elemental solids, substitutionally disordered alloys, surfaces, interfaces and grain boundaries, and impurities of substitutional or interstitial kinds in such materials. The formalism presented in this part is of necessity only a small part of the vast literature in this field, and unavoidably reflects the author's biases and particular preferences as to the line of development followed. At the same time, a number of references are given in the bibliography sections of the chapters from which the reader can obtain alternative points of view and formalisms.

In keeping with the aim of addressing this book to a student audience, a fairly large number of problems has been included. These problems hopefully will help clarify some of the concepts presented in the text, supplement others and above all may infuse the reader with a certain amount of confidence in the use of Green functions. In particular, it is hoped that the reader will attempt to construct at least a few of the fairly simple computer codes asked for in the problem sections. It may turn out to be pure pleasure to hold in one's hands finished codes based, say, on the coherent potential approximation, some of which can be shorter than one page in length.

At this point, I would like to express my gratitude to those friends, collegues and collaborators who in more ways than one have contributed to the completion of this project. I would like to begin by acknowledging my indebtedness to my thesis advisor and friend, James W. Garland, under whose tutelage began my forays into the territory of Green functions and multiple scattering theory. Other colleagues, G.M. Stocks, J.S. Faulkner, W.H. Butler, D.M. Nicholson, B.L. Györffy, R. Zeller and P. Dederichs, to name but a handful, have helped shape my ideas and have contributed encouragement and much moral support to carry out some of the work represented in the following pages. When I found myself out of work entirely upon the folding of the small community college in Chicago where I used to teach, A.J. Freeman provided me with a post-doctoral appointment at Northwestern University that essentially got me back into the track of practicing physics. And it was at Northwestern University that this book was begun and essentially completed. Finally, P.A. Sterne reviewed critically the entire manuscript and made numerous and substantive suggestions for improvement.

Regarding the completion of the manuscript, I would be hard pressed to express adequately my gratitude to Jean Shedd who supervised the typing of the original version, and of the two revisions that followed during the nearly five years that this project was in progress.

Arlene Jackson has done a superb job in the actual typing of the material. And last, but certainly not least, the editorial staff at North-Holland have worked tirelessly toward the production of the final, published version. It is hoped that their efforts and mine will not have been in vain and I thank them from the bottom my heart.

A. Gonis
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Pleasanton, CA

Contents