Planewaves, Pseudopotentials and the LAPW Method

Second Edition

PLANEWAVES, PSEUDOPOTENTIALS AND THE LAPW METHOD

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This book is dedicated to our wives, Nancy and Hedvig, whose love, patience and understanding made this work possible.

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Preface

The first edition of this book, published in 1994, provided an exposition of the LAPW method and its relationship with other electronic structure approaches, especially Car-Parrinello based planewave methods. Since publication of that book, the LAPW method has been transformed from a specialized method used mostly by researchers running their own home made versions, to a popular, widely used method, where most users run standard codes to investigate materials of interest to them. This is an exciting development because it opens the door to widespread use of first principles calculations in diverse areas of condensed matter physics and materials science. The positive impact of this on scientific progress is already becoming clear. Also as a result of this trend, the great majority of researchers using the LAPW method are no longer directly involved in the development of LAPW codes. Nonetheless, it remains important to understand how the LAPW method works, what its limitations are, and how its parameters determine the quality and efficiency of calculations. The scientist with an understanding of how the method works has a clear advantage. This edition is an updated and expanded treatment of the LAPW method, including descriptions of key developments in the LAPW method since 1994, such as $p_{1/2}$ local orbitals, the APW+LO method, LDA+U calculations and non-collinear magnetism, as well as much of the material from the first edition.

The exceptionally high accuracy and reasonable computational efficiency of the general potential linearized augmented planewave (LAPW) method has led to its emergence as the standard by which density functional calculations for transition metal and rare-earth containing materials are judged. Furthermore, the widespread availability of high quality, user-friendly LAPW codes has made it a very popular method for first principles studies of materials.

However, even though codes are generally provided in source form, it remains difficult for most users to delve into the method and implement calculations for properties of interest to them or simply to understand exactly how to set the parameters to optimally solve a given problem. Among the main obstacles

is the fact the essential details about the LAPW method are scattered through the literature, and some crucial aspects such as how to set the linearization parameters and sphere radii are hardly discussed at all. Newcomers to the field have had to learn the LAPW method either from one of the groups that currently uses it, or by the arduous process of reconstructing the method after gathering and digesting the literature on it.

This book has two primary purposes. The first is addressed in the main part of this book, which is aimed at lowering this barrier so that newcomers can quickly learn the method and start performing calculations using an existing code, or, if desired, write a new code without having to "reinvent the wheel". An algorithmic approach is used to do this. Theory is discussed, but the emphasis is on how a practical implementation proceeds and on information that will be useful in carrying out calculations with LAPW codes. It is our hope that this edition will help new researchers more effectively use the LAPW method and its extensions to solve problems of particular interest to them, as well as advancing the method by providing a unified exposition of its inner workings.

Our second purpose in writing this book derives from the very rapid progress in planewave based electronic structure techniques since the development of the Car-Parrinello method. These and related approaches have greatly increased the range of systems that can be treated using planewave based methods, but the underlying ideas have been slow to be applied to other methods. It is our view that this will prove to be a very fruitful endeavor. Accordingly, we devote a portion of this book to discussion of the (1) relationships between the LAPW and planewave pseudopotential methods, (2) essential aspects of the Car-Parrinello method and (3) early work aimed at incorporating Car-Parrinello like algorithms into the LAPW method. We hope that this will both help readers understand the relationship between different electronic structure methods and stimulate further work in this area.

The ideas presented in this book regarding the relationships between LAPW and pseudopotential methods have been evolving for some time, and are the product not only of our thinking, but that of many others as well. We have benefited greatly from contributions of others and from many helpful discussions that we have had the opportunity to participate in. We especially thank Henry Krakauer, who taught one of us (DJS) the LAPW method and Warren E. Pickett who served as his mentor at the Naval Research Laboratory. A substantial part of this book is composed of things learned from them. Special thanks are also due to Karlheinz Schwarz and to Peter Blaha. Many of the insights in this book derive from ongoing interactions with them and from especially discussions in Vienna and at a series of workshops in Planneralm, Austria. Thanks are also due to R.E. Cohen, S. Goedecker, C. Haas, B.M. Klein, D.D. Koelling, A.Y. Liu, I.I. Mazin, V.L. Moruzzi, M. Posternak, E. Sjöstedt, S.H. Wei, E. Wimmer and R. Yu.

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David J. Singh and Lars Nordström,