Theory of Single and Multiple Interfaces

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The Method of Surface Green Function Matching

Theory of Single and Multiple Interfaces

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To Carmen and Mercedes.

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PREFACE

This book is based on our personal experience with Green function calculations for matching problems of various kinds. For a number of years we have been developing and adapting the method of Surface Green Function Matching (SGFM) as new needs appeared in our own work on surfaces, interfaces, layered systems, quantum wells and superlattices. This required sometimes differential calculus - continuous systems - and others finite differences - discrete systems -, involving in all cases very different physical problems and normal modes or elementary excitations of a diverse nature. We have found in the SGFM method both a satisfactory formalism providing a unified view of apparently very different problems and a practical method for doing calculations.

There is unfortunately a rather widespread prejudice against Green functions which is totally unjustified. Perhaps the trouble is that most of us learnt Quantum Mechanics from textbooks written in terms of wavefunctions. The Green function is a very transparent concept which can be viewed as a propagator or as a response function and which is equally clear and meaningful all the way from classical physics to ordinary quantum mechanics down to the most intricate manybody quantum field theory. Not only that. It is also a very useful object to do practical calculations. It is simply not true that a Green function calculation is more complicated and one could find many test cases which bear this out. Yet we find sometimes this prejudice among very respectable colleagues who insist on this view. We respectfully submit that they have not tried.

In writing this book we have also been guided by comments, questions and response from many colleagues. This has helped us to detect the points where readers are likely to find obscurities and want clarification. The didactic tone of some passages, the explicit derivations almost step by step of some of the key results, the reflections on some elementary questions and the choice of some very simple examples selected to bear out basic points are our response to this very stimulating input we have received from many

people. Anyone engaged in research knows how difficult it is sometimes to give an honest answer to the usual question: where can I find this?. We always seem to manage to stumble upon our results in the clumsiest possible way and then it is very difficult to recommend in good faith any of the lousy papers we have written. These are for experts in the field, who can see their way through the increasing pollution in the current scientific literature, but not for those who are looking for an introduction to the field and want to learn the subject in order to use it in their own work. It is the latter that we have in mind as potential readers. So, having been doing SGFM calculations for a number of years we felt it was time to try and collect together our thoughts on the matter, enjoying the rare pleasure of pausing to meditate, and making an effort to put all these things together in one volume so we can give one reference when we are asked. If someone feels disappointed then this will only reflect our inability to do better. But we have tried.

In order to avoid interruptions in a continuous line of argument, which we feel is a more appropriate style for a book, we have listed the references by chapters at the end. We hope to have done justice to other authors and present our sincere apologies if someone has been unintentionally left out.

It is a pleasure to express our gratefulness to Ignacio Reguera for helping us in the preparation of the text with his bottomless magician's bagful of tricks.

This book owes a great deal to the work of some of our coworkers. M. Carmen Muoz has contributed very substantially to the practical development of the SGFM method for discrete systems. The whole of Chapter 7 would have been impossible without the decisive collaboration of Rolando Pérez-Alvarez and Huberto Rodríguez-Coppola. It is a pleasure to acknowledge here how much we owe to Carmen, Rolando and Huberto and it is impossible to express the deep human satisfaction and reward that their friendship and collaboration have meant to us. We also owe a great deal to many other friends and colleagues with whom we have been privileged to collaborate and whom it is impossible to name here one by one. Most of these come from parts of the world where to do anything at all is sometimes a miracle. In expressing here our gratitude to all of them we would like to manifest our respect and admiration for the many colleagues who, in the middle of all the problems and difficulties of less fortunate countries, strive for their dignity and for a place in the sunshine.

Madrid, December 1991.

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