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Jonas Fransson

Non-Equilibrium Nano-Physics

A Many-Body Approach

Springer

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I want to climb this ladder up to the stars
I feel no fear, from this height
Though there's no rescue in sight
A hollow yearning, and nothing learning
An ancient look at the watch on my wrist
My life has just been dismissed

I'm about to die, and I think I will
Have nothing left to loose, as I never had any skill

Preface

At some point earlier I would probably have named this book *f-electron methods applied to nanoscale systems*, which is a formally correct statement, however, it feels less relevant nowadays. Why? Because, although it is appealing to make the connection to the tradition of strongly correlated electron system and related issues, there are many questions traditionally considered in a textbook on strong electron correlations, that will not be covered within the present text. The intention with this book is not give an account of strongly correlated systems as such. Rather, the intention is to present a formulation of the non-equilibrium physics in nanoscale systems in terms of many-body states and operators and, in addition, discuss a diagrammatic approach to Green functions expressed by many-body states. Thus, the issues focused on in this book are results of typical questions that arise when addressing nanoscale systems from a practical point of view, e.g. current-voltage asymmetries, negative differential conductance, spin-dependent tunneling, local vibrations, and coupling to superconducting leads.

The use of many-body states and operators constructed of such states was previously introduced by, e.g. Hubbard 1963, but others have preceded him and many more will doubtlessly pick up ides along those lines. It is my aim to give a reasonable introduction to a formalism of non-equilibrium Green functions (NEGFs) expressed in terms of many-body operators. It is, however, more interesting to provide meaningful reasons for considering and using many-body states and many-body operator Green functions (MBGFs) in studies of localized electrons interacting with a de-localized environment. The strengths of any method based on many-body states becomes best visualized in systems where the localized electrons interact via e.g. Coulomb repulsion, hopping/tunneling, and exchange, and where the energy scales of these interactions are comparable. In other words, in systems where it does not make sense to pick out a single energy scale and consider it large in comparison with the others, it is often preferable to transform the localized subsystem into, e.g. its many-body eigenstates. Such a formulation gives a freedom in varying the energy scales of the localized subsystem without worrying about their mutual relationship. In short, the focus will be on nanoscale systems constituted of complexes of subsystems interacting with one another, under non-equilibrium conditions, in which

the local properties of the subsystems are preferably being described in terms of its (many-body) eigenstates.

Although the content of this book is discussed from the perspective of the physics, the book may still be considered as a book on a technique, or combinations of techniques. The discussion above mentions the many-body operator Green functions, which will be introduced and discussed at length. The discussion will, however, be focused on non-equilibrium conditions, which means that only little space will be spent on special techniques that may be used under strict equilibrium conditions. For those interested in strongly correlated electrons in the equilibrium case I refer to the excellent book by Ovchinnikov and Val'kov. Here, the technique will, thus, be set in the framework of non-equilibrium Green functions (NEGFs) and the formalism developed by Kadanoff and Baym, and Keldysh.

In order to develop a systematic approach that we can both apply to non-equilibrium conditions while still being efficient in the treatment of correlated states, one should be working with imaginary time contour ordered averages of operators. This enables a systematic diagrammatic expansion of our averages, expansions that usually are necessary to conduct in the class of systems under considerations. The diagrammatic expansions discussed here, are outlined by means of functional differentiations of averages.

My aim is that this book can be read by graduate students that have some experience in quantum mechanical field theory, Dirac formalism, second quantization, and quantum statistical methods. I certainly hope that experienced researcher will take up this book as well. Much of the content will be presented in a basic language, such as equation of motion and expansions, and I will not go into the deeper aspects given in a path integral approach. With this said, I thus hope that the present text will be accessible to many more readers that only to those who have a very deep fundamental understanding of the intricate world of quantum field theory.

The organization of this book is thought of as a bit evolutionary, in the sense that it begins with a class of problems where one encounters problems when working with conventional field theoretical methods. Then, the concept of many-body states and many-body operators is introduced and the Green functions are constructed and discussed. Only after this, the systems are being simplified in order to better illustrate the technique itself. This is meant to turn focus on the technique rather than on the complexity of the physical system. As the concepts are becoming familiar we can again add complexity

Finally, it is with a great pleasure I thank I. Sandalov for teaching me about non-equilibrium, Green functions, many-body operators, and strongly correlated electron systems. I would also like to thank A.V. Balatsky and J.-X. Zhu for introducing me into STM techniques and spin dynamics in non-equilibrium. Further, I am grateful to M. Galperin for sharing his views on extensions of the Hubbard operator scheme to include electron-vibron coupled systems. My Ph.D. student P. Berggren has done a good job in proof reading parts of the text, for which I thank him. I am indebted to O. Eriksson and L. Nordström for being understanding and patient with my questions, discussions, and ideas concerning correlated electron systems and the use of Hubbard operators in various possible and impossible instances. Last but not

least, I want to express my gratitude towards my wife Johanna, and my children Eugenia, Elmer, Wilbur, and Werner, which have been and still are tremendously patient with me.

Uppsala Jonas Fransson

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