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Long and short time quantum dynamics: I. Between Green's functions and transport equations

Václav Špička[a,*], Bedřich Velický[a,b], Anděla Kalvová[a]

[a] Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 182 21 Praha 8, Czech Republic
[b] Faculty of Mathematics and Physics, Charles University, Ke Karlovu 2, Praha 2, Czech Republic.

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Abstract

This paper summarizes the present views on construction of the electron quantum transport equations based on the Non-Equilibrium Green's Functions approach. The basic tool is the so-called Ansatz decoupling; one Ansatz family stems from the original Kadanoff-Baym Ansatz and is suitable for extending the quasi-particle picture of the Landau theory out of equilibrium. The other family based on the Generalized KB Ansatz is appropriate for short time transients. The physical and formal context of the Ansatzes is analyzed; the most important question explored is the status of the Reconstruction Theorems, reducing a full description of a non-equilibrium system to a dynamic theory in terms of one-particle quantities. A comparison is made between the Time Dependent Density Functional Theory and the properly renormalized NGF formalism. There is a close relationship between both formalisms. The Reconstruction Theorems form a general basis for obtaining improved quantum transport equations.

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1. Introduction

This paper is the first one of three contributions to this volume ([1], hereafter called Paper II, [2], hereafter called Paper III) devoted to quantum transport out of equilibrium, that is to say, beyond the linear response. We concentrate on a specific question of generating reliable transport equations for electrons in extended systems driven by external fields under various conditions which might be broadly divided into "slow" and "fast" phenomena, represented by quasi-stationary quantum transport, and optical or transient processes, respectively. We need to describe both regimes properly. As the underlying general description of non-equilibrium systems, we will use the Non-equilibrium Green's Functions (NGF) [3–9] – double-time correlation

*Corresponding author.
E-mail address: spicka@fzu.cz (V. Špička).

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functions which include full quantum sub-dynamics of interactions in the presence of arbitrary external fields and/or in highly non-equilibrium transient states. The NGF can be used to describe actual systems directly, but we presently discuss the methods of an approximate reduction of the theory to equations for single-time quantities, quantum distribution functions. The approximations are based on hierarchy of characteristic times of a given system and they all have "Ansatz" in their name with reference to the original, so-called Kadanoff–Baym Ansatz (KBA) [3,8].

In agreement with the above division of phenomena to slow and fast, the basic formalism forks into two specific lines of developing single-time evolution equations. The common "intuitive" tool to describe transport experiments (long time behavior) is a quantum generalization of the Boltzmann equation (BE) [3–12]. It is based on the concept of a quasi-particle distribution function and on the quasi-classical approximation suitable if everything varies smoothly in space and time. In the NGF context, the mild time dependence, in particular, is a necessary condition for the validity of the KBA, which has been devised to obtain the quantum generalizations of the Boltzmann equation. We will call this type of evolution equations the Quantum Kinetic Equations (QKE). Further progress in this direction led to an extension of the Ansatz incorporating off-shell propagation in an effective manner. The resulting modified scheme has been used to obtain the quantum BE with the corresponding corrections [6,13–15].

If a smooth time dependence cannot be assumed, a more complete quantum treatment becomes necessary to describe the short time (transient) and high-frequency processes. For states far from equilibrium, a theory interpolating adequately between the fully quantum linear response (…the standard Kubo formula, whose use is limited to weak external fields acting on an equilibrium system) and the quasi-classical high-field BE is needed. Such a theory may be based on the quantum Generalized Master Equations (GME) [8,9,16,12] with a strictly causal structure. These equations abandon the quasi-particle distribution concept and describe the evolution of the density matrix (or Wigner function) for true particles. The tool for generating the GME within the NGF environment is a correspondingly structured Ansatz usually called Generalized KB Ansatz (GKBA) [17–20,8,9]. Also this Ansatz can be further developed and refined to obtain an improved GME with a wider range of applicability [8,9].

It is remarkable that more than 40 years since the inception of the KBA, and almost 20 years since its modification to the GKBA, this area of non-equilibrium physics is still active and developing, as witnessed by the number of papers and of meetings devoted to it [21–23]. The questions addressed range from the practice of employing the quantum transport equations to the justification, extension and refinement of the Ansatz-based bridge between the NGF and other quantum transport approaches. These problems are the subject matter of the present paper series.

It should be stressed that similar questions and tasks emerge in very small metal and semiconductor systems. Quantum coherence plays an essential role in the behavior of such systems. A natural question emerges to how the behavior of such systems corresponds to the "classical" way of description known from classical thermodynamics and statistical physics. We attempt to describe a unifying approach to non-equilibrium dynamics, which, while based on studies of extended systems, is also well suited for systems with a reduced dimensionality.

Summary of Papers I, II, III

This Paper I and the adjoining Papers II, III are not intended as an exhaustive review. They rather try to stress the basic issues from our point of view. This is especially true of this first one. The subject matter is divided roughly as follows. In this paper, we present an overview of the basic concepts and of the formal means used. The paper culminates in the last section devoted to the *reconstruction problem*: to what extent can the non-equilibrium dynamics of the many-particle system be described in terms of the evolution of the one-particle distribution? Paper II is devoted to the case of the quasi-particle transport in quasi-classical