



Contents lists available at SciVerse ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop



Physical scales in the Wigner–Boltzmann equation

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ARTICLE INFO

Article history:

Received 14 May 2012

Accepted 2 October 2012

Available online 9 October 2012

Keywords:

Wigner–Boltzmann equation

Quantum transport

Decoherence

Scattering

ABSTRACT

The Wigner–Boltzmann equation provides the Wigner single particle theory with interactions with bosonic degrees of freedom associated with harmonic oscillators, such as phonons in solids. Quantum evolution is an interplay of two transport modes, corresponding to the common coherent particle-potential processes, or to the decoherence causing scattering due to the oscillators. Which evolution mode will dominate depends on the scales of the involved physical quantities. A dimensionless formulation of the Wigner–Boltzmann equation is obtained, where these scales appear as dimensionless strength parameters. A notion called scaling theorem is derived, linking the strength parameters to the coupling with the oscillators. It is shown that an increase of this coupling is equivalent to a reduction of both the strength of the electric potential, and the coherence length. Secondly, the existence of classes of physically different, but mathematically equivalent setups of the Wigner–Boltzmann evolution is demonstrated.

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1. Introduction

The Wigner theory establishes a phase space formulation of quantum mechanics, where both states and observables are represented by functions of coordinates and momenta. Many notions of classical

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statistical mechanics such as probability distributions and mean values are retained in this picture, which recovers physical intuition in the field of quantum theory. Historically introduced with the help of the Schrödinger equation [1,2], modern Wigner theory represents an independent formulation, recognized as equivalent and autonomous alternative to operator mechanics [3]. The formalism has been further applied to scattering problems within the basic particle–potential interaction, and beyond, to multiple scattering problems [4]. With the introduction of additional degrees of freedom, which need to be eliminated by corresponding averaging, the single particle state ceases to be pure, so that irreversibility and effects of decoherence begin to characterize the evolution of the particle state.

The problem of environmentally induced decoherence of quantum systems to semi-classical states has been a subject of intensive research over the past three decades [5,6]. In particular, the concept of einselection of pointer states has been very successful in explaining the general behavior of quantum particles subjected to decoherence effects both from a fundamental point of view [7,8] and in solid-state nanostructures such as open quantum dots [9]. The Wigner function is recognized as a convenient formalism to study these processes theoretically [8,10], or experimentally [11]. Recently, the application of quantum physics to information theory has enlarged the interest in sources and time scales of decoherence processes as part of the efforts to develop devices for quantum processing of signals. Decoherence effects may even have a strong influence on the behavior of more conventional nanoscaled solid-state devices [12]. In this field the Wigner formalism is nominated as a legitimate inheritor of the classical solid-state electron transport model, as it provides an extension of the latter for kinetic processes occurring in nanoscale devices [13], which is demonstrated by simulations of a variety of transport conditions in actual devices like RTD's and DG-MOSFET's [14] and of the scattering-induced decoherence in semiconducting nanostructures [15].

In this way the problem of exploring the gap between quantum-coherent and scattering dominated evolution modes has both fundamental and practical aspects. The physical system chosen for this purpose presents solid state electrons moving in a given electric field and interacting with lattice vibrations, described in terms of harmonic oscillators—phonons. While the approach applied in the following remains general, the concrete system allows to regard phonons as a thermostat—an environment which causes decoherence without being affected by the electron subsystem. This allows to perform averaging and to obtain the Wigner–Boltzmann (WB) equation for the electrons where the environment participates with well-defined Bose equilibrium averages.

The fundamentals of the equation can be traced back to certain uniform field transport models, which utilize the Wigner formalism to derive classical [16], or quantum-mechanical [17] electron–phonon interaction operators. The Wigner equation augmented by a Boltzmann-like collision operator has been suggested for the case of general potentials as an intuitive deduction from these models [18–20]. It has been demonstrated that phase-breaking and energy dissipation processes are needed to maintain the physical behavior of the modeled system [21,22]. Thus, initially, the Boltzmann-like phonon collision operator acting upon the Wigner quasi-distribution is an a priori, but necessary assumption that 'is an adequate approximation at some level' [21]. What are the physical conditions allowing the common existence of the classical scattering operator next to the quantum Wigner-potential operator? The answer is not trivial: derivations from first principles and analysis of the assumptions and approximations have been provided only recently for interactions with ionized impurities [23] and with phonons [24]. Relations between spatial, energy and time scales are specified by theories which turn out to be relevant to the transport conditions in modern nanoelectronic devices.

As implied by the name of the Wigner–Boltzmann equation, the two limiting regimes of coherent or classical transport are obtained by setting one of the corresponding operators to zero. They have rather opposing roles in determining the properties of the solution.

If the coupling with the phonons becomes negligible, two different situations may occur. If the electric potential changes up to quadratically within the spatial extension of the electron wave packet, the electron is a particle with a ballistic evolution along classical Newton's trajectories. Otherwise the kinetics are quantum-coherent. The electric potential causes oscillations and negative values, around abrupt potential changes in regions of tunneling and quantization [25]. These features are the manifestations of the quantum character of the Wigner function even for the simple situation of an initial state resulting from a superposition of two Gaussian wave functions [5]. In this case, oscillations

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