Master Equations in Quantum Transport

Irena Knezevic
Electrical and Computer Engineering, University of Wisconsin-Madison, USA
e-mail: knezevic@engr.wisc.edu

In the theory of small, few-level open systems, the term "master equation" refers to equations that describe the evolution of the open system's full statistical operator (usually called the reduced statistical operator or the reduced density matrix) in the presence of coupling with reservoirs, which have an infinite number of degrees of freedom and are responsible for the irreversibility in the open system's evolution [1,2]. Traditionally, the reservoirs are considered bosonic and can have various spectral function [1], although the question of small open systems coupled with fermionic reservoirs has been receiving a lot of attention in recent years [3].

Electronic systems in semiconductor nanostructures are open quantum systems, exchanging particles and information with the contacts, rapidly dephasing reservoirs of charge. The term master equation is somewhat more broad when referring to electronic transport calculations. On the one hand, we have few-level models (e.g. the resonant-level models used for quantum dots) for which master equations continue to refer to the dynamics of the full reduced statistical operator [4,5]. On the other hand, if we strive to account for the generally continuous single-particle spectrum of an electron in a nanostructure (e.g. when capturing current in structures without resonances) and the fact that many electrons are available to populate them, then calculating the full many-body reduced statistical operator becomes both intractable and unnecessary, as much information can be obtained from the single-particle quantities. In this case, master equations can refer to the equations for the time evolution of the single-particle density matrix (e.g. Redfield-type equations [6] or generalized semiconductor Bloch equations [7]), its Wigner transform (i.e. the Wigner equation [8]), or just its diagonal terms (e.g. the Pauli master equation [9]).

Master equations as used in quantum transport in nanostructures can be divided in two groups based on the treatment of the interaction with the contacts: Markovian equations, in which just the current state of the contacts plays a role (obtained in the weak-coupling limit, large-bias limit, or singular coupling limit) and non-Markovian equations, in which details of the contact evolution over a finite time in the past affects the state of the open electronic system. Non-Markovian (also known as memory) effects are critical in resolving the short-time dynamics of electronic systems, such as in the interaction of electrons with ultrafast electromagnetic fields or when looking at the fluctuations of charge and current.

In this talk, I will review recent progress on the use of various Markovian and non-Markovian master equations in quantum transport. I will discuss issues such as complete positivity of the map when deriving approximations for master equations, the relationship between master equations and diagrammatic techniques, and address some of the problems that stem from the separation of contacts from the active region and tracing out of the contact degrees of freedom.

I will also present work [10] on completely positive non-Markovian dynamics in two terminal structures that can be obtained based on the approximation of rapid relaxation in the contacts due to electron-electron scattering. Self-consistent coupling of the Schrödinger equation, Poisson equation, continuity equation, and a master equation obtained by coarse-graining over the contact relaxation time results in non-Markovian transient response of nanostuctures, such as a silicon *nin* diode (Fig. 1) or a GaAs/AlGaAs tunneling diode (Fig. 2).

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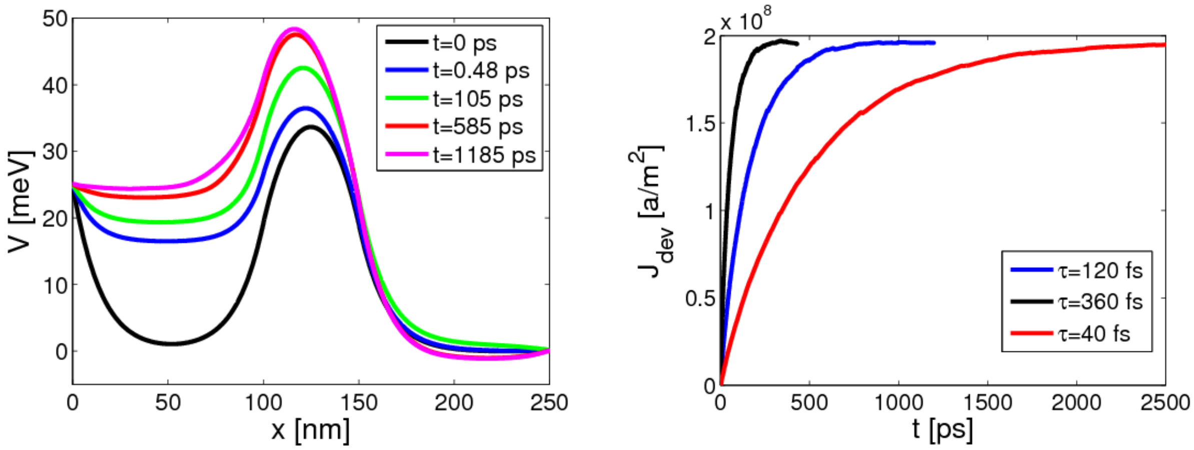

Fig. 1: (Left) Time evolution of the potential profile in a silicon *nin* diode. (Right) Transient current in the active region of the *nin* diode for different values of the momentum relaxation time in the contacts [10].

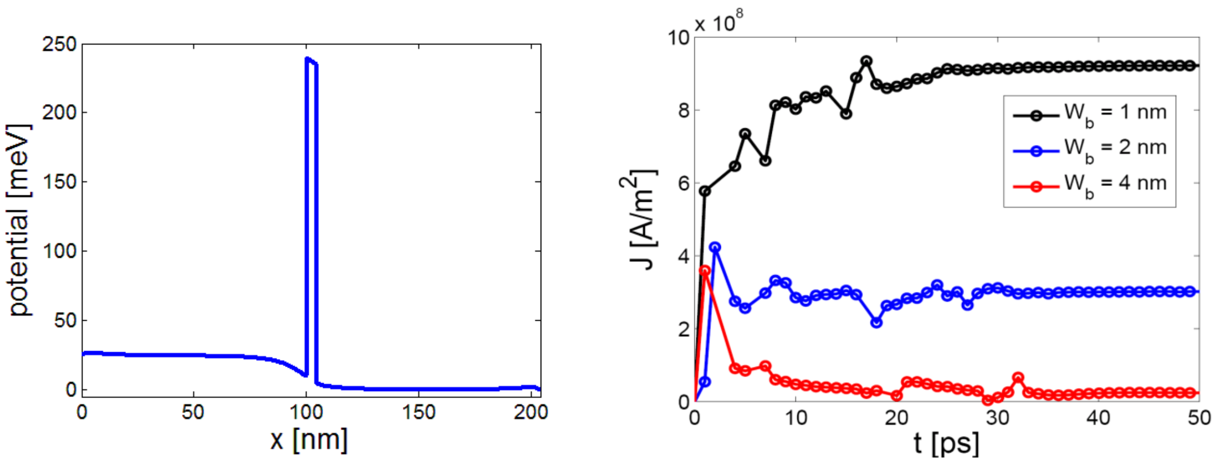

Fig. 2: In a GaAs/AlGaAs tunnel barrier (potential profile in left panel), the finite time needed to empty the well to the left of the barrier, connected to the relaxation time in the contacts, affects the shape of the transient (right).