Ballistic Electron Transport Described by Higher-Order Schrödinger equations

Giulia Elena Aliffi* Giovanni Nastasi† Vittorio Romano‡

Abstract

A fourth-order Schrödinger equation for charge transport in semiconductors operating in the ballistic regime is introduced, incorporating non-parabolic effects in the dispersion relation and thereby going beyond the simple effective-mass approximation. As in the standard second-order formulation, the problem is confined to a finite spatial domain and equipped with transparent boundary conditions to simulate charge transport in a quantum coupler, where an active device region is connected to leads acting as reservoirs. Several analytical properties of the model are established, and a new expression for the current is derived. Numerical results highlight the main qualitative features of the solutions. In particular, interference effects appear due to the richer wave structure induced by the fourth-order formulation—effects absent in the effective-mass approximation. Building on this approach, a hierarchy of models is further developed, each governed by a Schrödinger equation of progressively higher order. Several analytical properties of these generalized models are analyzed and a unified current formula valid for any order is derived. Numerical simulations of a resonant tunneling diode (RTD) demonstrate the impact of the generalized formulation on device behavior.

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*University of Catania, Department of Mathematics and Computer Science, Catania, Italy (giuliaelena.aliffi@phd.unict.it).

†University of Enna "Kore", Department of Engineering and Architecture, Enna, Italy (giovanni.nastasi@unikore.it).

‡University of Catania, Department of Mathematics and Computer Science, Catania, Italy (Corresponding author: vittorio.romano@unict.it).

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