Robust design of quantum potential profile for electron transmission in semiconductor nanodevices

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***Abstract*— In this paper we address the robust design of the quantum potential profile in a in semiconductor nanodevice to achieve a desired electron transmission coefficient vs. bias voltage characteristic despite uncertainty. We formulate an optimization problem which is solved locally via a sequential linear program.**

"What I want to talk about is the problem of manipulating and controlling things on a small scale.
As soon as I mention this, people tell me about miniaturization, and how far it has progressed today. They tell me about electric motors that are the size of the nail on your small finger. And there is a device on the market, they tell me, by which you can write the Lord's Prayer on the head of a pin. But that's nothing; that's the most primitive, halting step in the direction I intend to discuss. It is a staggeringly small world that is below. In the year 2000, when they look back at this age, they will wonder why it was not until the year 1960 that anybody began seriously to move in this direction."
– Richard P. Feynman, "There's Plenty of Room at the Bottom," American Physical Society, Caltech, Dec. 29, 1959

I. Introduction

There is equal "wonder" looking back from this end of the time tunnel that Feynman was able to herald nanotechnology so many years ago. With the development of more sophisticated fabrication and control techniques, it is only now that it has become possible to create semiconductor devices with dimensions at several nanometers. Examples of such devices include quantum dots [6], nanowires [1], and electron gas in GaAs-AlGaAs heterostructures [10]. For semiconductor devices of this size, many quantum-mechanical wave effects can be observed such as tunneling and nonequilibrium behaviors. Such effects are may be critical in the design of new electronic devices.

There are at least two generic quantum design problems which can stated in the form of an optimization problem. In both cases we start with a model Hamiltonian operator, $H(\theta, u, w)$, with design parameters $\theta \in \Theta$, input variables $u \in U$, and uncertain parameters $w \in W$. The output variables are given by the measurement rule of quantum mechanics, *i.e.*, $y(\theta, u, w) = \langle\psi|O|\psi\rangle$ where O is the observable operator and $|\psi\rangle$ is the quantum state which solves the time-independent Schrödinger equation associated with the Hamiltonian. A typical optimization problem in this context is as follows:

$$\min_{\theta\in\Theta} \max_{u\in U,\ w\in W} \left\| y(\theta, u, w) - y^{\mathrm{des}}(u) \right\| \tag{1}$$

where $y^{\mathrm{des}}(u)$ is the desired input/output relation. This "input/output" design problem arises in many cases where the device is to exhibit a particular characteristic impedence, voltage/current relation, *etc.*. This problem has been previously addressed in [9] to achieve a desired transmission profile and in [2] to make a layered semi-conductor to achieve desired quantum wells. In these cases exhaustive numerical searches were used to find solutions. This takes enormous computing time and the search space grows exponentially as the dimension of the problem increases. In this paper we address the application in [9] as an optimization problem in the form of (1). In [4] an optimizing potential design was developed for a similar electron transmission problem restricted to a single input voltage.

Another generic problem is to design the device to achieve a characteristic spectrum. In this case the optimization problem would look like,

$$\min_{\theta\in\Theta} \max_{u\in U,\ w\in W} \left\| \lambda\left\{H(\theta, u, w))\right\} - \lambda^{\mathrm{des}}(u) \right\| \tag{2}$$

where $\lambda^{\mathrm{des}}(u)$ is the desired spectrum as a function of the applied input. This problem is also referred to as an Inverse Eigenvalue Problem and has been adderessed extensively, *e.g.*, [5], [3]. Atom placement to achieve a desired spectrum is an example [11] where again an exhaustive numerical search is performed.

A. In this paper

Solving these types of problems may lead to software design tools to explore the design of new devices which utilize quantum phenomenon. In this paper, we consider (1) for designing quantum potentials for electron transmissions in semiconductor devices. For an electron at a given energy transporting through a quantum potential in a semiconductor device, its transmission coefficient can be described as a function of the applied external bias voltage. Our objective is to design a quantum potential such that the electron transmission achieves a prescribed transmission coefficient vs. bias voltage characteristics, e.g., a linear or quadratic function. In practice, the quantum potential in a semiconductor device may be generated laterally, e.g., with a one-dimensional grating potential constructed by electron-beam lithography; or vertically, e.g., by varying the composition of an $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ alloy in the epitaxial growth processes. In addition, we seek a robust potential design that is tolerant to parameter uncertainty as might arise from manufacturing errors. We employ a Monte Carlo based optimization procedure by generating a large number of samples which numerically

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characterize the statistics of the parameter uncertainty. Using a sequential linearization we then solve a linear programming problem at each iteration to find a local solution.

B. Some typical solutions

The goal is to design the quantum potential profile that achieves as close as possible a specified linear transmission coefficient vs. bias voltage relation despite dielectric uncertainty. A nominal potential profile, shown in Figure 2(A), is designed assuming no uncertainty and yields a relative RMS error of 0.0188. The transmission coefficients achieved by this initial potential is plotted in Figure 2(B). We now apply the robust optimization algorithm starting with this potential and assuming a 1% level of (relative) dielectric uncertainty. The resulting robust quantum potential profile is shown in Figure 2(C). For no uncertainty this potential has a relative RMS level of 0.0149, and its transmission-voltage curve is shown in Figure 2(D). Suprisingly the nominal (no uncertainty) RMS level of the robust potential is better than the the RMS level of several of the potential optimized with no uncertainty! The reason for this is an on-going research effort. Our current speculation is that this type of problem is essentially identicle to the quantum state-to-state transfer problem addressed in [8], [7].

In Figure 1, the top plot shows the histogram of RMS error distributions for initial potential and the bottom plot the histogram for the robust potential. The dashed line indicates the 90th percentile. It is clear that the robust quantum potential reduces the RMS errors in the case when dielectric constants are not precisely known.

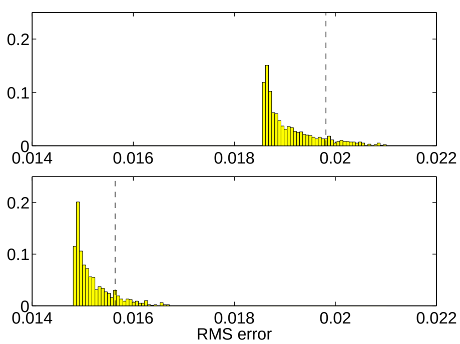

Fig. 1. Histograms of RMS error distributions for initial potential (top) and robust potential (bottom) for a 1% dielectric error. The vertical dashed line marks the 90th percentile.

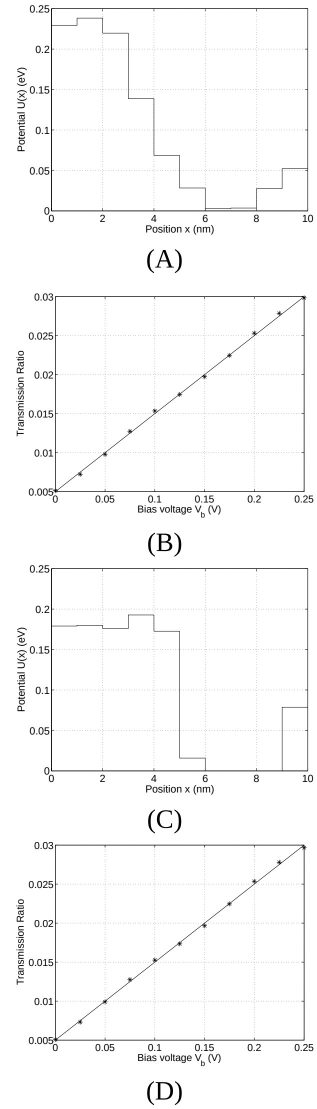

Fig. 2. Robust quantum potential design result. (A) Initial potential profile;(B) Transmission-voltage curve achieved by the initial potential; (C) Potential profile from robust design; (D) Transmission-voltage curve achieved by the robust design.

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