Comparison between Pseudospectral and Discrete Geometric Methods for Modelling Quantization Effects in Nanoscale Electron Devices

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***Abstract*— This paper aims at comparing Pseudospectral method and Discrete Geometric approach for modelling quantization effects in nanoscale devices. To this purpose, we implemented a simulation tool, based on both the methods, to solving self-consistent Schrödinger-Poisson coupled problem for a 1D electron gas according to Effective Mass Approximation model (suitable for FinFETs and nanowire FETs).**

***Index Terms*— Schrödinger-Poisson problem, Pseudospectral method, Discrete Geometric approach.**

I. Introduction

The success of the MOS technology over the last thirty years has been determined by its scaling capability. Nowadays, the silicon technology is approaching the physical limits of the traditional bulk MOS devices: therefore, new device architectures like silicon nanowire FETs and fin-shaped FETs (FinFETs) could represent a valid alternative to conventional bulk planar MOSFETs [1]. Thus, an accurate and yet computationally efficient description of the carrier quantization in these devices is an important modeling target. In the electron device community the numerical modelling of such a problem is frequently tackled by solving a coupled Schrödinger-Poisson problem, using Finite Difference (FD) or Finite Elements (FE) methods. The simulation of arbitrarily shaped domains, like those of real electron devices, is problematic with FD methods; on the contrary, FE methods provide an accurate geometric representation but leads to a discrete counterpart of Schrödinger problem in terms of a computationally heavy generalized eigenvalue problem.

The aim of this paper is to explore more efficient discretization approaches, with respect to FD and FE, for self-consistent solution of Schrödinger-Poisson coupled problem in the case of a 2D carrier confinement, relevant for nanowire FETs and FinFETs. In the full paper, we will present a systematic comparison between the numerical efficiency of Pseudospectral methods (PS) [3], [6] and Discrete Geometric approach (DG) [4], [5]. The PS and DG methods are benchmarked in terms of CPU time, geometric modelling capability, by inspecting their accuracy in terms of not only subband energies but also electron concentration distributions.

II. Quantization in nanodevices

The geometry of interest for a cylindrical nanowire FET is shown in Fig. 1A. Quantization problem occurs on a bi-dimensional domain $D = D_{ch} \cup D_{ox}$ on a plane (y, z) normal to the transport direction x, where D_{ch}, D_{ox} denote the channel and oxide domains respectively (see Fig. 1B); the surrounding gate electrode is modelled as an equipotential

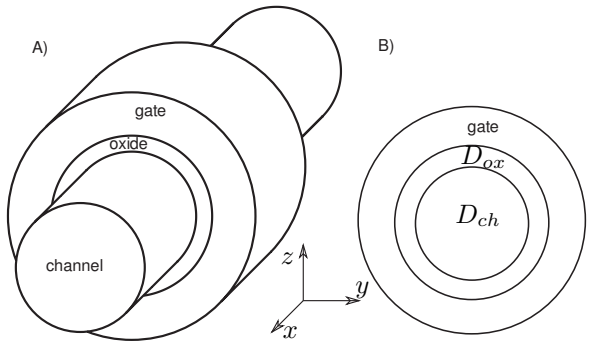

Fig. 1. On the left: Device coordinate system (x, y, z) for a cylindrical nanowire FET. On the right: Device cross-section normal to the transport direction x, where the domain of interest $D = D_{ch} \cup D_{ox}$ is depicted.

domain. In order to compute the electron density in narrow nanowires and FinFETs, the Effective Mass Approximation (EMA) model is typically adopted to describe quantization phenomena in domain D [2]; this leads to the following 2D Schrödinger equation in D

$$-\mathrm{div}\, \mathrm{q}_\nu(\mathrm{r})\, \mathrm{grad}\Psi_{\nu,j}(\mathrm{r}) + U(\mathrm{r})\Psi_{\nu,j}(\mathrm{r}) = \lambda_{\nu,j}\Psi_{\nu,j}(\mathrm{r}), \quad (1)$$

where ν is the valley[1] index, r is the position vector of a point $r = (y, z) \in D$ and $\partial/\partial x = 0$ holds; $\Psi_{\nu,j}(\mathrm{r})$ denotes the wave function corresponding to the j-th eigenvalue $\lambda_{\nu,j}$ and $\mathrm{q}_\nu(\mathrm{r})$ is a double tensor, whose Cartesian components in D are the inverse of effective masses for each valley index ν. Finally, potential energy $U(\mathrm{r})$ of an electron can be expressed as

$$U(\mathrm{r}) = -e\phi(\mathrm{r}) - \chi(\mathrm{r}), \quad (2)$$

where $\phi(\mathrm{r})$ is electric scalar potential describing the electrostatic behavior of the nanodevice, e is the absolute value of electron charge and $\chi(\mathrm{r})$ is the prescribed medium dependent energy affinity of the electron in D. Interface condition in D and boundary conditions on ∂D must be added to (1), in order to well pose the problem.

The electrostatic behavior of nanodevices can be modelled by coupling to Schrödinger problem (1) a Poisson problem for the electric scalar potential $\phi(\mathrm{r})$

$$-\mathrm{div}\, \epsilon(\mathrm{r})\, \mathrm{grad}\phi(\mathrm{r}) = -e(N_A^-(\mathrm{r}) + n(\mathrm{r})),\ \mathrm{r} \in D, \quad (3)$$

where $\epsilon(\mathrm{r})$ denotes medium permittivity double tensor, $N_A^-(\mathrm{r})$ denotes concentration of ionized acceptor atoms, that is null in D_{ox}, and $n(\mathrm{r})$ denotes electrons concentration in the conduction band. Again boundary and interface conditions must be added to close Poisson problem (3).

[1] A valley denotes a conduction-band energy minimum.

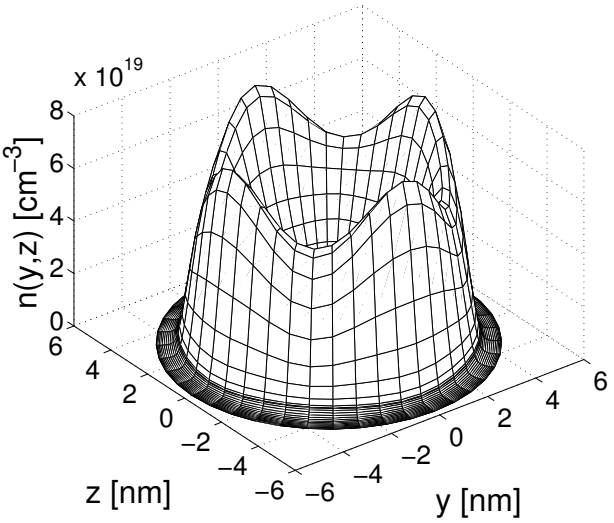

Fig. 2. Electron concentration $n(y,z)$ for a cylindrical nanowire obtained with PS method in the effective mass approximation.

The coupling between Schrödinger (1) and Poisson (3) problems is two fold. On the one hand, electric scalar potential $\phi(\mathrm{r})$ determines potential energy $U(\mathrm{r})$ in (2). On the other hand, concentration $n(\mathrm{r})$ of electrons in the conduction band in (3) is given by $n(\mathrm{r}) = \sum_\nu \sum_j N_{\nu,j} |\Psi_{\nu,j}(\mathrm{r})|^2$, where $N_{\nu,j}$ is a known prescribed function of eigenvalue $\lambda_{\nu,j}$ [7].

III. Discretization and numerical results

We discretized Schrödinger (1) - Poisson (3) coupled problem, according to PS [3] and DG methods [4], [5]; we provide here a summary of the idea at the base of each methodology, all the details will be given in the full paper.

PS method approximates unknown function of a differential problem or of an eigenvalue problem by using algebraic or trigonometric polynomials. Provided that a grid of nodes is introduced in D, using an appropriate coordinate transformation based on polar coordinates [6], derivatives of unknown function at each grid node are approximated with those of the approximating polynomial. The resulting discretization matrices are not sparse, but PS method can achieve the so called *spectral accuracy*[2].

On the other hand, DG approach puts the spot of the light on the geometrical structure behind a physical theory [5]. According to this approach, we developed a novel discrete geometric formulation of Schrödinger equation in terms balance equations; such balance equations involve integral variables associated with precise geometric elements of a pair of two-dimensional interlocked cell complexes in D, one dual of the other, the primal being based on simplexes. We deduced, in a purely geometric way, a computationally efficient discrete counterpart of Schrödinger problem (1) in terms of a *standard* symmetric eigenvalue problem with diagonal matrix on the right hand of the eigenvalue problem [4]. Computationally, this is a big advantage compared with Finite Elements, where a symmetric *generalized* eigenvalue problem is obtained instead, which is notoriously heavy to be computed and can be numerically unstable. Moreover, boundary and interface conditions together with non homogeneity and anisotropy of the media involved in D can be accounted for in a straightforward manner. Finally, we also reformulated the Poisson problem (3) according to DG approach, yielding to a sparse algebraic system of equations. In this way, we obtained a discrete counterpart of the overall Schrödinger-Poisson coupled problem.

We solved the coupled problem for a cylindrical nanowire with d=10nm and a $[100]$ transport orientation. A doping density N_A=$1 \times 10^{15}\mathrm{cm}^{-3}$, a gate voltage $V_G = 0.6V$, an equivalent oxide thickness of $0.7\mathrm{nm}$ and a gate work function ϕ_m=$4.05\mathrm{eV}$ have been considered in these preliminary simulations. Electron concentration $n(y,z)$, obtained with PS method, is shown in Fig. 2 for example; a similar result is obtained with DG approach. The electron concentration is clearly anisotropic, reflecting the anisotropy of the electron energy dispersion. In order to obtain an efficient convergence of the Schrödinger-Poisson loop, we employed the so called non-linear formulation of the Poisson equation described in [7].

IV. Conclusions

A comparative analysis, whose results will be presented in the full paper, confirmed that Pseudospectral methods can achieve the spectral accuracy but are mainly suitable for simple geometries. On the contrary, Discrete Geometric approach allowed to handle more complex and general 2D and 3D geometries. Both the techniques yield to a standard matrix eigenvalue problem instead of a generalized one like in Finite Elements as concerns the discrete counterpart of Schrödinger problem.

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[2]The spectral accuracy consists of an exponential reduction of the approximation error according to c^N, with N being the degree of the polynomial and $c \in (0,1)$.