Geometry of the 3D Schrödinger problem and comparison with Finite Elements discretization

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***Abstract*—The numerical modeling of nanoscale electron devices needs the development of accurate and efficient numerical methods, in particular, for the numerical solution of the Schrödinger problem. If Finite Elements methods allow an accurate geometric representation of the device, they lead to a discrete counterpart of Schrödinger problem in terms of a computationally heavy *generalized* eigenvalue problem. Exploiting the geometric structure behind the Schrödinger problem, we will construct a numerically efficient discrete counterpart of it, yielding to a *standard* eigenvalue problem. We will also show how the two approaches are only partially akin each other even when lumping is applied.**

***Index Terms*—nanoelectronics, semiconductor device modeling, Schrodinger equation, finite elements method**

I. Introduction

Modern microelectronics and optoelectronics use semiconductor materials structured at truly nanometric dimensions [1]; as an example, the silicon technology is now approaching the physical limits for the traditional bulk MOS devices, since the carrier transport is confined in very thin semiconductor layers and new device architectures like silicon nanowire FETs and fin-shaped FETs (FinFETs) are under investigation as valid alternatives [2].

The modeling of such nanoscale electron devices is based on multi-physics simulations, where transport equation or electrostatics are coupled with Schrödinger equation [3]. Still, solving the Schrödinger problem is the key bottleneck of the simulation; thus, we focus on the development of accurate and efficient numerical methods for the solution of the Schrödinger equation in the *effective mass* approximation [4].

In this framework, one of the purposes of the paper is to show how the geometric structure behind the Schrödinger problem, formulated in arbitrarily 3D shaped domains, leads to a numerically efficient discrete counterpart consisting of a *standard* eigenvalue problem. Such a result follows from the so-called Discrete Geometric Approach (DGA) [5]. On the contrary, Finite Elements (FE) discretization yields to a computationally heavy *generalized* eigenvalue problem.

Moreover, we will also show how the discrete counterpart of the Schrödinger problem, deduced from DGA, and that from FE are partially related by a lumping technique. Finally, a numerical comparison between the two discrete counterparts is also given in terms of convergence with mesh refinement and accuracy.

II. The Schrödinger equation reformulated

We focus on a 3D spatial domain D, individuated by the Cartesian components (x, y, z) of the position vector r (vectors and tensors are denoted in roman type) of a particle; the medium properties are described by a diagonal double tensor q(r) whose ij-th Cartesian component, with $i, j = 1, \dots 3$, is

$$q_{ij}(\mathrm{r}) = \frac{\hbar^2}{2m_i(\mathrm{r})}\delta_{ij}, \tag{1}$$

where $\hbar$ is the reduced Plank constant and $m_i(\mathrm{r})$ is the *effective mass* coefficient of the particle, along the i-th Cartesian axis, with $i = 1, \dots 3$; δ_{ij} is the Kronecker symbol. We also denote with λ the unknown eigenvalue (or energy level) and with $\psi(\mathrm{r})$ the corresponding eigenfunction evaluated at a point r; $m_i(\mathrm{r})$ is here assumed independent of λ. Finally, $u(\mathrm{r})$ denotes the confinement potential energy term in D, considered known in this paper. Now, we introduce a pair of vector fields a(r), b(r) and a scalar field $\phi(\mathrm{r})$ in such a way that

$$-\mathrm{grad}\,\psi(\mathrm{r}) = \mathrm{a}(\mathrm{r}), \tag{2}$$

$$\mathrm{div}\,\mathrm{b}(\mathrm{r}) = \phi(\mathrm{r}) \tag{3}$$

and

$$\mathrm{q}(\mathrm{r})\mathrm{a}(\mathrm{r}) = \mathrm{b}(\mathrm{r}), \tag{4}$$

$$(\lambda - u(\mathrm{r}))\psi(\mathrm{r}) = \phi(\mathrm{r}), \tag{5}$$

hold simultaneously. Of course, boundary conditions on ∂D and interface conditions must be considered in addition to close the problem. It is apparent that (2), (4), (3) and (5) are equivalent to the standard time independent Schrödinger problem [4]

$$-\mathrm{div}\,\mathrm{q}(\mathrm{r})\mathrm{grad}\,\psi(\mathrm{r}) = (\lambda - u(\mathrm{r}))\,\psi(\mathrm{r}). \tag{6}$$

III. The discrete geometric eigenvalue problem

According to the Discrete Geometric Approach, using a pair of interlocked cell complexes with V tetrahedra and N nodes, we will demonstrate how a discrete counterpart of the Schrödinger problem based on a piecewise uniform approximation of ψ can be written as

$$(\mathbf{S} + \bar{\mathbf{U}})\,\bar{\mathbf{\Psi}} = \bar{\lambda}\bar{\mathbf{T}}\,\bar{\mathbf{\Psi}}, \tag{7}$$

where, the array $\bar{\mathbf{\Psi}}$, of dimension N, contains the nodal values of ψ, the square matrices $\mathbf{S}$, $\bar{\mathbf{U}}$, $\bar{\mathbf{T}}$ have dimension N and

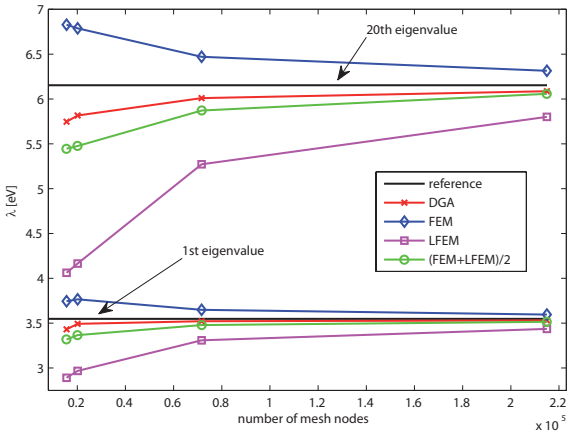

Figure 1: The convergence w.r.t. mesh refinement of the first and twentieth eigenvalues.

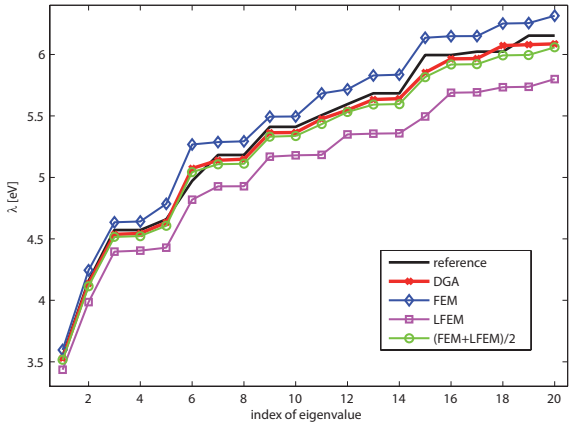

Figure 2: The first twenty eigenvalues on the finest mesh.

their entries are strictly related to the metric of the geometric elements of the primal complex; moreover the entries of $\bar{\mathbf{U}}$ are deduced using an affine approximation of $u(\mathrm{r})$ in D and the metric of the dual complex. An important result of the geometric discretization approach is that $\bar{\mathbf{T}}$ is diagonal; thus (7) can be easily and efficiently transformed into a *standard* eigenvalue problem.

IV. FE generalized eigenvalue problem and lumping

According to the FE method [6] based on the affine approximations of $\psi(\mathrm{r})$ and of $u(\mathrm{r})$ in D, the discrete counterpart of the Schrödinger problem yields the following *generalized* eigenvalue problem

$$(\mathbf{S}_{FE} + \mathbf{U}_{FE})\,\mathbf{\Psi}_{FE} = \lambda_{FE}\mathbf{T}_{FE}\,\mathbf{\Psi}_{FE}, \tag{8}$$

where the array $\mathbf{\Psi}_{FE}$ of the $\psi(\mathrm{r})$ values has dimension N and the square matrices $\mathbf{S}_{FE}$, $\mathbf{U}_{FE}$, $\mathbf{T}_{FE}$ have dimension N. We will demonstrate that $\mathbf{S}_{FE} = \mathbf{S}$ holds; however, the matrix $\mathbf{T}_{FE}$ is not diagonal and to transform (8) into a standard eigenvalue problem, it is usual to apply the so called lumping technique [6] to the matrix $\mathbf{T}_{FE}$, yielding

$$(\mathbf{S}_{FE} + \mathbf{U}_{FE})\,\mathbf{\Psi}_{l} = \lambda_{l}\,\mathbf{T}_{l}\,\mathbf{\Psi}_{l}, \tag{9}$$

where the lumped matrix $\mathbf{T}_l$ is diagonal, with entries $(\mathbf{T}_l)_{ii} = \sum_{j=1}^{N}(\mathbf{T}_{FE})_{ij}$ for $i = 1,\ldots,N$. Moreover, in the full paper we will demonstrate how lumping technique applied to the FE matrix $\mathbf{T}_{FE}$ yields the matrix $\bar{\mathbf{T}}$ from discrete geometric approach and we write $\mathbf{T}_l = \bar{\mathbf{T}}$.

V. Numerical results

The formulations have been integrated into the GAME (Geometric Approach to Maxwell's Equations) Fortran 90 code developed by the Authors. The FEAST [7] library has been employed to solve the discrete eigenvalue problems.

To validate the results produced by the described formulations and compare them, a particle in a box benchmark—which admits a pseudo analytical solution using pseudospectral methods [2]—has been analyzed. This benchmark consists of a cube of edge $d = 10$ nm in which the energy distribution $u(\mathrm{r}) = x + y + z\,\mathrm{eV}$ is assumed, where x, y, z range from 0 to 10 nm, and q is a homogeneous, anisotropic diagonal tensor $\mathrm{q} = \mathrm{diag}(0.04159, 0.20053, 0.20053)$.

In Fig. 1, the convergence w.r.t. mesh refinement of the first and twentieth eigenvalues computed by DGA, Finite Elements (FEM) and lumped Finite Elements (LFEM) is compared. Obviously, the same mesh is used for all the considered methods. Moreover, the mean between FEM and LFEM is also considered, since these formulations provide upper and lower bounds for eigenvalues [6].

The DGA exhibits superior accuracy w.r.t. FEM and LFEM techniques and this behavior holds for all eigenvalues, as Fig. 2 shows for the first twenty. DGA is advantageous also from the execution time point of view, since a standard eigenvalue problem is solved in place of a generalized one. In fact, generalized eigenvalue problem solvers need stiffness matrix factorization, that is extremely memory and time consuming for large scale problems. Three other problems whose results confirm the advantages of DGA will be presented in the full paper, demonstrating the convenience of DGA with respect to FEM both in terms of accuracy and speed.

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