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Detailed numerical simulation of nanoelectronic devices

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G. Iannaccone, "*Detailed numerical simulation of nanoelectronic devices*", Nano et Micro Technologies, **3**, pp.133-142 (2003).

Waveforms usable for digital clock signal have also been recently obtained (Seabaugh *et al.*, 1999) with very simple circuitry.

4. Discussion

The resonant tunnelling diode is an extremely interesting device from the point of view of understanding transport in highly confined structures, and for circuit applications. At present, research mostly focuses on transport and noise in the presence of strong magnetic fields, and on silicon-based resonant interband tunnelling diodes, that have the great advantage of being easily integrable with CMOS technology.

5. References

Chang L. L., Esaki L., Tsu R., "Resonant Tunneling in semiconductor double barriers", *Appl. Phys. Lett.*, Vol. 24, 1974, pp. 593-595.

Iannaccone G., Lombardi G., Macucci M., Pellegrini B., "Enhanced Shot Noise in Resonant tunneling: Theory and Experiment", *Phys. Rev. Lett.*, Vol. 80, 1998, pp. 1054-1057.

Iannaccone G., Pellegrini B, "Compact formula for the density of states in a quantum well", *Phys. Rev. B*, Vol. 53, 1996, pp. 2020-2025.

Iannaccone G., Pellegrini B, "Unified approach to electron transport in resonant tunneling diodes", *Phys. Rev. B*, Vol. 52, 1995, pp. 17406-17412.

Jonson M., Grincwaig A., *Appl. Phys. Lett.*, Vol. 51, 1987, pp. 1279-1281.

Luryi S., "Frequency limit of double barrier resonant tunneling oscillators", *Appl. Phys. Lett.*, Vol. 47, 1985, pp. 490-492.

Mazumder P., Kulkarni S., Bhattacharya M., Sun J. P., Haddad G. I., "Digital Circuit Applications of Resonant Tunneling Diodes", *Proc. IEEE*, Vol. 86, 1998, pp. 664-686.

Seabaugh A., Brar B., Broeakaer T., Morris F., var der Wagt P., Frazier G., "Resonant-Tunneling Mixed-Signal Circuit Technology", *Solid State Electronics*, Vol. 43., 1999, pp. 1355-1365.

Seabaugh A., Deng X., Blake T., Brar B., Broekaert T., Lake R., Morris F., Frazier G., "Transistors and tunnel diodes for analog/mixed-signal circuits and embedded memory", *IEDM Technical Digest*, pp. 429-432.

Stone A. D., Lee P. A, "Effect of inelastic processes on resonant tunneling in one dimension", *Phys. Rev. Lett.*, Vol. 54, 1985, pp. 1196-1199.

Sun J. P., Haddad G. I., Mazumder P., Schulman J. N, "Resonant Tunneling Diodes: Models and Properties", *Proc. IEEE*, Vol 86, 1998, pp. 641-661.

Tsu R, Esaki L., "Tunneling in a finite superlattice", *Appl. Phys. Lett*, Vol. 22, 1973, pp. 562-564.

Van Der Wagt, "Tunneling-based SRAM", *Proc. IEEE*, Vol. 87, 1999, pp. 571-595.

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ABSTRACT. Issues related to the numerical simulation of nanoelectronic devices are addressed, with particular reference to the approach adopted in the EU funded project NANOTCAD. Basics of numerical simulation are described, as well as the structure of the 2D and 3D codes for the simulation of semiconductor devices developed within the NANOTCAD project. Reference is provided to typical simulation results, to additional material and to possibility of using the NANOTCAD codes, with sample input files and complete user's manuals on the PHANTOMS simulation hub.

KEYWORDS: noise, nanoelectronics, shot noise, mesoscopic devices, ballistic MOSFETS.

1. Introduction

The development of novel devices at the nanometer scale with potential for large-scale integration and room temperature operation is a formidable task. Over the years, many ideas have been proposed on the basis of very qualitative reasoning or simplified physical models: typically, the demonstration of working prototypes is achieved, while the fabrication of complex logic circuits proves to be unfeasible. There are often fundamental problems, such as the extreme sensitivity of device operation to the presence of defects, stray charges, and other parasitics, or the need of prohibitively tight fabrication tolerances. In other cases the switching times are inherently slow, or the physical effect is so weak that room temperature operation is prevented.

Many of the difficulties and of the limits of candidate technologies for nanoelectronics and molecular electronics could be predicted, anticipated and, hopefully, solved if detailed modeling tools of realistic devices and structures were available. The same modeling tools could be used to design more robust devices, and to select molecules and device structures with potential for use in large-scale integrated circuits.

The importance of Computer Aided Design (CAD) tools in the development of industrial semiconductor technology is well outlined in the 1997 edition of the SIA National Technology Roadmap for Semiconductors – Technology Needs (page 6): "Modeling and simulation is the only tool available for engineers to design processes, material use, transistors, and structures; there is no viable alternative. The major challenge is getting predictive model results from atomic scale through electrical performance; to accurately model new technologies a priori, resulting in development cost reduction; and faster time to market."

2. Basics of numerical device simulation

Nanoelectronic devices are typically characterized by strong charge confinement in at least one dimension, and by an intrinsic three-dimensional nature. For these reasons, a simulation tool aiming at addressing a broad range of devices must have the capability of solving the Poisson-Schrödinger equation in three dimensional domains. An approach based on the envelope function approximation, and on Density Functional Theory (DFT) with local density approximation has been adopted. While the limitations of such approach are apparent (Macucci *et al.*, 2001), it still provides the best trade-off between numerical complexity and accuracy, for the vast majority of devices of interest.

Without loss of generality we shall refer to simulation of two-dimensional semiconductor structures, as has been implemented in the NANOTCAD2D code (Curatola *et al.*, 2003).

The Poisson equation in two dimension reads:

$$\nabla\cdot\left[\varepsilon\nabla\phi(\vec{r})\right]=-q\left[-n(\phi)+p(\phi)-N_A^-(\phi)+N_D^+(\phi)\right], \qquad [1]$$

where ϕ is the electric potential, ε is the dielectric constant, n and p are the electron and hole densities, respectively: in the quantum region they are obtained by solving the Schrödinger equation with density functional theory, in other regions are given by the corresponding semiclassical expressions; N_A^- and N_D^+ are the ionized acceptor and donor concentrations, respectively. The Schrödinger equation in two dimensions for electrons, within the envelope function approximation, reads:

$$-\frac{\hbar}{2}\left[\frac{\partial}{\partial x}\frac{1}{m_{sx}}\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\frac{1}{m_{sy}}\frac{\partial}{\partial y}\right]\Psi_s+E_{Cs}\Psi_s=E_s\Psi_s, \qquad [2]$$

where Ψ is the wavefunction, $\hbar$ the reduced Planck's constant, E_C the confinement potential energy (conduction band plus exchange-correlation term), m_x (m_y) the effective mass in the x (y) direction, and the subscript s denoted the conduction band minimum being considered. Indeed, for direct gap materials such as GaAs it is sufficient to solve (2) only once, putting $m_{1x}=m_{1y}=m_{1z}=0.067m_0$, with m_0 the electron mass at rest; for indirect gap materials such as silicon, instead, Equation [2] must be solved once for each couple of minima in the conduction band, therefore s=1,2,3, and we have for s=1: $m_{1x}=m_l$, $m_{1y}=m_{1z}=m_t$; for s=2: $m_{2y}=m_l$, $m_{2x}=m_{2z}=m_t$; for s=3 $m_{3z}=m_l$, $m_{3x}=m_{3y}=m_t$, where m_l (m_t) is silicon longitudinal (transversal) effective mass.

Once the Schrödinger equation is solved, electron concentration is given by:

$$n=2\sum_s\frac{\sqrt{2m_{sz}k_BT}}{\pi\hbar}\sum_i\left|\Psi_{is}(x,y)\right|^2F_{-\frac{1}{2}}\left(\frac{E_{is}-E_F}{k_BT}\right), \qquad [3]$$

where k_B is the Boltzmann constant, T the temperature, E_F the Fermi energy.

Partial differential equations [1] and [2] must be *discretized*, *i.e.*, translated into algebraic non linear equations, in order to be solved numerically. First, we have to define the simulation domain, the region in which the equation must be solved, and the grid, *i.e.*, a finite set of points belonging to the domain in which we want to compute the values of the equation unknowns. Then, equations can be discretized with the *box integration* technique, if we observe that both (1) and (2) are of the form $\nabla\cdot\vec{f}=g$. Indeed, we can define the subdomain ΔS_i around the generic point i of the grid, as shown in Figure 1, and integrate both terms of the equation in the subdomain, using Gauss-Green theorem for the left-hand side. We have:

$$\iint_{\Delta S_i} \nabla \cdot \vec{f} dS_i = \int_{\partial S_i} \vec{f} \cdot d\vec{l} = \iint_{\Delta S_i} g dS_i \cdot \qquad [4]$$

Then, by considering f constant on each side of ΔS_i and g constant in the subdomain, we obtain

$$\sum_j \bar{f}(M_j) \cdot \partial l_{i,j} = \Delta S_i \cdot g_i \cdot \qquad [5]$$

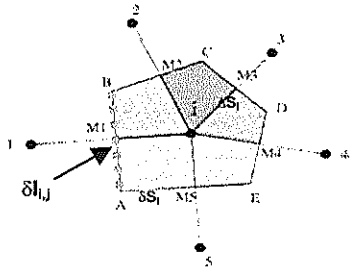

Figure 1. *Subdomain ΔS_i around the generic grid point i for box integration*

As mentioned the procedure can be applied both to the Poisson equation and to the Schrödinger equation.

3. Nanoscale device simulation in the NANOTCAD codes

3.1. *3D Poisson-Schrödinger solver*

In the codes developed within the NANOTCAD project (nanotcad.iet.unipi.it), a Poisson-Schrödinger solver with good scalability properties for large grids has been developed, based on a multigrid algorithm. Multigrid methods are known to solve elliptic partial differential equations discretized on N grid points in $O(N)$ operations (Press *et al.*, 1992), and offer several advantages with respect to the Newton-Raphson algorithm. First, multigrid methods are known to converge in a number of step smaller than any other "rapid" method (like, for example, Fourier or reduction methods (Press *et al.*, 1992). In addition, they have reduced memory requirements: while the Newton-Raphson method requires the Jacobian matrix to be stored ($7N$ elements), in the multigrid method only arrays of size N have to be stored. The non-linear Poisson equation can be discretized with the box integration method on several grids of different size, from the finest (of order 10^5-10^6 points) to the coarsest (a 3x3x3 grid).

The structure of the multigrid algorithm is sketched in Fig. 2. "E" represents the exact solution on the 3x3x3 grid, the rising line "I" represents the interpolation on the next-finer grid, "S" represents the "smoothing" operation, *i.e.*, a series of relaxation steps based on the Newton-Raphson algorithms which basically reduce the residue, the descending line "R" represents restriction on the next-coarser grid, and "L" represents smoothing plus solution of the Schrödinger equation. Without loss of generality, Figure 2 refers to a problem with 4 different grids, where grid 1 is the finest and grid 4 the coarsest.

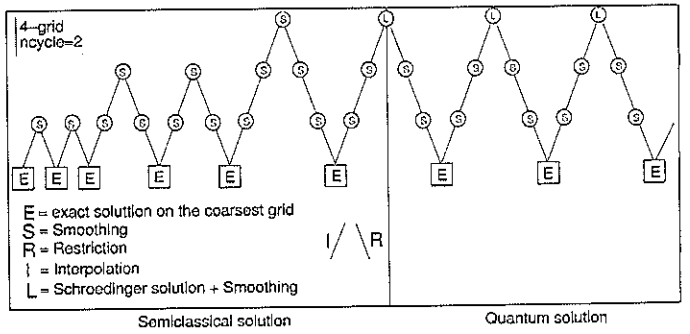

Figure 2. *Structure of the Poisson-Schrödinger solver based on the multigrid algorithm. The case of four different grids is represented*

First, the approach consists in solving the non-linear Poisson equation with a semiclassical approximation starting from an initial solution on the coarsest grid (3x3x3 points), where the Poisson equation is a single-variable nonlinear equation. The method then consists of a fixed number of steps on different grids, called V-cycles from the recursive restriction and interpolation steps. The solution on each grid is found by adding a corrector term obtained by solving the equation on a coarser grid to an approximate solution, obtained by means of relaxation cycles based on the Newton-Raphson algorithm. The mathematical details of the method can be found in (Press *et al.*, 1992).

The potential obtained at the end of the semiclassical cycle is used as an initial guess of the solution of the Poisson-Schrödinger equation. Then, a new number of V-cycles and relaxation steps is set for the following part of the algorithm. Every time the algorithm is at the top of a V-cycle (*i.e.*, on the finest grid), the Schrödinger equation is solved with DFT, and eigenfunctions are computed, restricted and stored on all grids. The V-cycle is then performed as already described, with the only difference that the electron density in the quantum region is computed from the stored eigenvalues.

Among several approaches to solve the Schrödinger equation (for example, Ritchie *et al.*, 1998, Trellakis 2000), a solver in the momentum space has been

developed (*k*-space) that will allow extension to full-band simulations. The basic idea is to transfer the eigenvalue problem to the *k* space by means of Fast Fourier Transform (FFT). The problem is then solved in the *k* space and the solutions are then transferred back to the real space by the anti-transform operator. The precision of results and the efficiency of the routine strictly depend on the choice of the basis in the *k* space. If the elements of the wave vector basis are a good approximation of the single particle eigenfunctions, then a small basis is sufficient to adequately describe the solution of the Schrödinger equation, even if in the real space a larger number of points are required to accurately reproduce the potential profile. To find the lowest eigenvalues a sub matrix has to be diagonalized corresponding to the smallest wave vectors. The advantage from the point of view of memory requirements (that scale as N^2) and of computing time (that scales as N^3 for a complete diagonalization, where N is the matrix order), is evident.

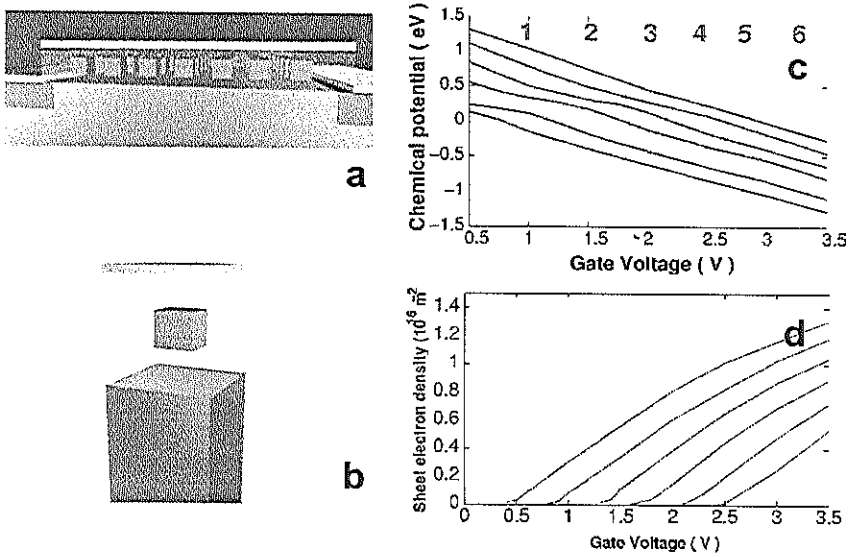

Figure 3. *Simulation of silicon nanocrystal memories with NANOTCAD3D: a) simplified structure of a nanocrystal memories, in which disorder in nanocrystal size and density has been removed; b) elementary periodic cell considered in the 3D simulation; c) chemical potential of the dot as a function of the voltage applied to the top gate for number of electrons in the dot ranging from 1 to 6; d) two-dimensional electron density at the Si-SiO2 interface as function of the gate voltage for an increasing number of electrons in the dot, from 0 to 5 (all figures from Iannaccone et al., 2001)*

Moreover, it is necessary to enforce Dirichlet boundary conditions on the eigenfunctions. In order to force the eigenfunctions to zero at domain boundaries, a

basis of only sine functions for the *k* space has to be used. The sine-FFT is used to compute the eigenfunction expansion in the sine basis. By solving the sub-matrix corresponding to smaller values of *k* it is then possible to gain efficiency without losing precision of the solutions for the lowest eigenvalues (Pala *et al.*, 2002).

Particularly interesting results have been obtained in the simulation of quantum dot flash memories, both in the silicon-silicon oxide and in the AlGaAs-InGaAs material systems, of single electron transistors, of silicon-germanium quantum wires and of ballistic field effect transistors. Figure 3 shows the typical structure of a silicon nanocrystal flash memories considered in a simulation and the relevant results as far as the stationary electrical properties of the device are concerned, i.e. chemical potentials and electron density in the channel as a function of the gate bias and of the number of electrons stored in the dots (Iannaccone *et al., 2001).*

3.2. *Modeling of ballistic field effect transistors*

As far as the simulation of nanoscale HFETs is concerned, the approach of considering "ballistic" electrons not just as a perturbation to a "normal", quasi-thermal electron distribution, but as mainstream electrons, has been adopted. As zero order approximation, fully ballistic transport has been considered.

Simulations of ballistic MOSFETs have been first performed by Natori (Natori 1994) by means of an analitical model. Moreover, recent simulations based on semiclassical Monte Carlo codes (Bude 2000) and on a scattering theory of MOSFETs (Lundstrom *et al.*, 2000) exhibit significant differences with respect to simulations based on drift-diffusion or energy balance models.

Nanoscale MOSFETs, in particular, exhibit a significant degree of quantum confinement in the channel: indeed, in order to control short channel effects, gate oxide thickness is reduced and bulk doping is increased, which in turn cause an high electric field in the vertical direction, confining electrons at the Si/SiO_2 interface. A quantum simulation is consequently required to take into account the 2D subband splitting and the lifting of the six-fold degeneracy of silicon conduction band minima. This is especially required to reproduce the experimental MOSFET threshold voltage V_T, since semiclassical simulation may underestimate V_T by more than 100 mV (Fiori *et al.*, 2002a).

Observing that quantum confinement is strong only along the direction perpendicular to the Si/SiO_2 interface, the Schrödinger equation can be decoupled into a 1D equation in the vertical direction (x) and a 1D equation in the longitudinal direction (y): the density of states in the y-direction is well approximated by the semiclassical expression, since there is no in-plane confinement, while discretised states appear in the vertical direction. Such approximation reduces has been shown to considerably the computational complexity of the problem, while introducing only a negligible error (Fiori *et al.*, 2002a). In order to obtain the I-V characteristics of the 25 nm nMOSFET, a fully ballistic model has been assumed for carrier

transport. In this way, current-voltage characteristics is reduced to a simple carrier transmission problem over the channel potential, which is represented by the edge of the subbands originated by the 1D-quantum confinement. Carriers with energy larger than the subband maximum can be transmitted from source to drain by thermoionic emission, while carriers with lower energy can travel along the channel only by tunneling. Since the tunneling component is negligible even in devices with channel length of 10 nm (Bude 2000, Pirovano *et al.*, 2002), initially quantum tunneling of the channel barrier has not been considered. The transmission coefficient has been then taken equal to unity above the maximum of the barrier and zero below. In this way electrons with energy smaller than the subband maximum energy are in thermal equilibrium with the closest contact (source or drain), while electrons with larger energy traverse the channel without energy loss. The electron concentration is computed by assuming that the states with energy below the maximum of the potential barrier have an occupation factor determined by the source/drain Fermi energy E_{fS} and E_{fD} respectively), while states with higher energy propagating from the source (drain) have the occupation factor of the originating contact (Fiori *et al.*, 2002b).

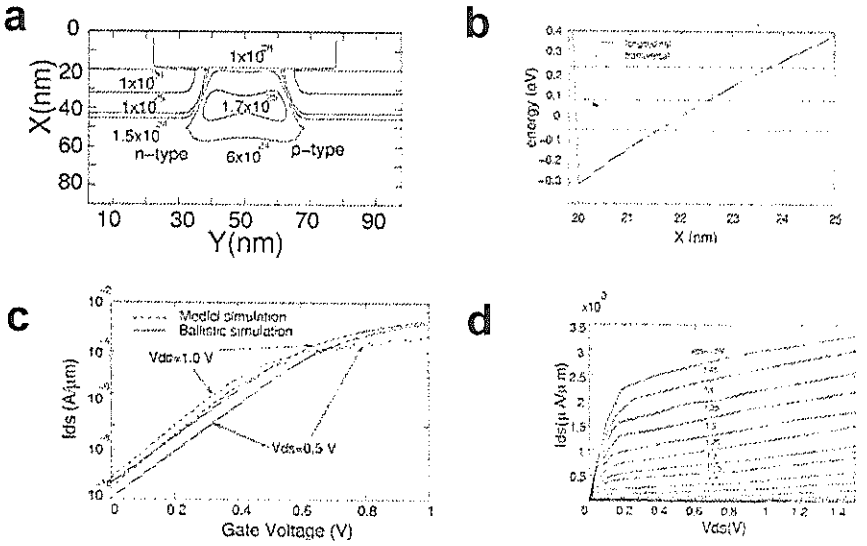

Figure 4. *Results from the simulation of the 25 nm "well tempered" MOSFET: a) doping profile of the device; b) conduction band profile and energy levels of the two-dimensional subbands in the middle of the channel, from which the very strong quantum confinement is apparent; c) comparison between the transfer characteristics computed with the ballistic code and those obtained from simulations with the commercial simulator Medici; d) output characteristics of the device [all figures from (Fiori et al., 2002b)*

Figure 4 shows results from (Fiori *et al.*, 2002b) obtained from the simulation of a so-called "well tempered" MOSFET with channel length of 25 nm, used as a benchmark structure for comparison of different simulation methods.

4. Conclusion

If nanotechnology will acquire industrial and economic relevance, it will strongly depend for its development on reliable Computer Aided Design tools, in the same way as Microelectronics relies upon TCAD tools. Within the EU funded NANOTCAD project (nanotcad.iet.unipi.it), three programs have been developed for the simulation of semiconductor nanostructures in quasi-equilibrium conditions in one-, two-, and three-dimensional domains (NANOTCAD1D, NANOTCAD2D, NANOTCAD3D, respectively). All codes are based on the solution of the many-body Schrödinger equation with density functional theory, local density approximation, and allow subdivide the domain in several regions with different types of quantum confinement, providing a reasonable level of flexibility. In addition, NANOTCAD2D also allows to simulate ballistic FET both in the III-V and in the Si-SiO2 material system.

All mentioned codes are freely usable on the PHANTOMS simulation hub (www.phantomshub.com) and can be remotely run by anyone connected to the internet. The hub also contains complete user's manuals and a set of sample input files for typical devices of interest.

5. References

Bude J. D. "MOSFET modelling into the ballistic regime", Proceedings of the International Conference on the Simulation of Semiconductor Processes and Devices (SISPAD) 2000, pp. 23-26.

Curatola G., Iannaccone G., *to be published on Computational Material Science*, 2003.

Fiori G., Iannaccone G., "Modeling of ballistic nanoscale metal-oxide-semiconductor field effect transistors", *Appl. Phys. Lett.* Vol. 81, 2002, pp. 3672-3674,

Fiori G., Iannaccone G. "The effect of quantum confinement and discrete dopants in nanoscale 50 nmn-MOSFETs: a three-dimensional simulation", *Nanotechnology* Vol. 13, 2002, pp. 294-298.

Lundstrom L., Ren Z., Datta S., "Essential Physics of Carrier Transport in Nanoscale MOSFETs", *Proceedings of the International Conference of the Simulation of Semiconductor Processes and Devices (SISPAD)* 2000, pp. 1.

Macucci M., Iannaccone G., Greer J., Martorell J., Sprung D.W. L., Schenk A., Yakimenko I. I., Berggren K.-F., Stokbro K., Gippius N., Nanotechnology, Vol. 12, 2001, pp. 136-142.

Natori K., "Ballistic metal-oxide-semiconductor field effect transistors", *J. Appl. Phys.* Vol. 76, 1994, pp. 4879-4890.

Pala M. G., Iannaccone G., Kaiser S., Schliemann A., Worschech L., Forchel A., "Extraction of parameters of surface states from experimental test structures", *Nanotechnology*, Vol. 13, 2002. pp. 369-372.

Pirovano A., Lacaita A., Spinelli A. S., "Two-dimensional quantum effects in nanoscale MOSFETs", *IEEE Trans. Electron Devices* Vol. 49, 2002, pp. 25-31.

Press W. H., Vettering W. T., Teukolsky S. A., Flannery B. P., *Numerical Recipes in Fortran 77: the art of scientific computing*, Cambridge University Press, Cambridge, 1992.

Ritchie B., Weatherford C. A., "Use of a Fast Fourier Transform (FFT) 3-D Time Dependent Schroedinger Equation Solver in Molecular Electronic Structure", *Int. J. Quantum Chem.* Vol. 70, 1998, pp. 627-635.

Trellakis A., Ph. D. dissertation, University of Illinois at Urbana-Champaign, 2000.

Noise in nanoelectronic devices

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ABSTRACT. *In this paper we present a brief review of properties of noise in nanoelectronic devices, focusing on shot noise, that is particularly relevant in nanoscale devices and when few electrons determine device behaviour. We review cases in which shot noise is significantly altered with respect to full shot noise, i.e., that associated to a Poissonian process, in order to gain insights into the details of the transport mechanisms. We focus both on mesoscopic (ballistic) devices at very low temperature and on more conventional MOSFETs at the nanoscale, that are entering mass production and, due to their small scale, exhibit noise properties similar to those observed in more exotic mesoscopic devices.*

KEYWORDS: *noise, nanoelectronics, shot noise, mesoscopic devices, ballistic MOSFETs.*