

COUPLED QUANTUM-CLASSICAL TRANSPORT IN SILICON NANOWIRES

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Key words: Silicon nanowires, Schrödinger-Poisson-Boltzmann system, hydrodynamic model, maximum entropy principle

Abstract. We present an extended hydrodynamic model describing the transport of electrons in the axial direction of a silicon nanowire. This model has been formulated by closing the moment system derived from the Boltzmann equation on the basis of the maximum entropy principle of Extended Thermodynamics, coupled to the Schrödinger-Poisson system. Explicit closure relations for the high-order fluxes and the production terms are obtained without any fitting procedure, including scattering of electrons with acoustic and non polar optical phonons. We derive, using this model, the electron mobility.

1 INTRODUCTION

Silicon nanowires (SiNWs) are quasi one-dimensional structures in which the electrons are spatially confined in the two transversal directions and free to move in the longitudinal one. SiNW devices have been fabricated recently using lithographic techniques [1]. They have attracted significant interest due to their potential to function as logic devices, thermoelectric devices, and sensors. Therefore, it is crucial to accurately model and estimate the performance of these devices.

By shrinking the dimension of electronic devices, effects of quantum confinement are observed and the wave nature of the electrons must be taken into account. The Non-Equilibrium Green Function formalism is the most advanced transport model for the simulation of SiNW devices, but it necessitates rather intensive computational efforts since it requires detailed information on the propagation of the electron wave packet injected in the device. Under reasonable hypothesis, transport in low-dimension semiconductors can be tackled coupling quantum and semiclassical tools. In fact, the main quantum transport phenomena in SiNW transistors at room temperature, such as the source-to-drain tunneling, and the conductance fluctuation induced by the quantum interference,

become significant only when the longitudinal length (called channel) is smaller than 10nm [2]. Therefore, for longer channels, semiclassical formulations based on the 1-D Multiband Boltzmann Transport Equation (MBTE) can give reliable simulation results when it is solved self-consistently with the 3-D Poisson and 2-D Schrödinger equations in order to obtain the self-consistent potential and subband energies and wavefunctions [1]. Another simplification comes from the use of the Effective Mass Approximation (EMA), which is supposed to be still a good solution in the confining direction in the presence of disorder, which is probably valid for semiconductor nanowires down to 5 nm in diameter, below which atomistic electronic structure models need to be employed. Solving the MBTE numerically is not an easy task, because it forms an integro-differential system in two dimensions in the phase-space and one in time, with a complicate collisional operator. The full solution of the MBTE can be obtained or by using the Monte Carlo (MC) method [3]-[10] or by using deterministic numerical solvers [11],[12],[13] at expense of huge computational times. Another alternative is to obtain from the MBTE hydrodynamic models that are a good engineering-oriented approach. This can be achieved by taking moments of the MBTE, and by closing the obtained hierarchy of balance equations as well as modeling the production terms (i.e. the moments on the collisional operator).

2 Transport equations

In the following we shall consider a SiNW with rectangular cross section. For a quantum wire with linear expansion in z-direction, and confined in the plane x-y, the normed electron wave function $\psi(x, y, z)$ can be written in the form

$$\psi(x, y, z) = \chi_\alpha(x, y) \frac{e^{ik_z z}}{\sqrt{L_z}} \quad (1)$$

where $\chi_\alpha(x, y)$ is the wave function of the α -th subband and the term $e^{ik_z z}/\sqrt{L_z}$ describes an independent plane wave in z-direction confined to the normalization length, where $z \in [0, L_z]$ and k_z is the wave vector number. In general the electron is subject to external confining potential U , such as by a discontinuity in the band gap at an interface between two materials, and also to the effect of the other electrons in the system. The simplest approximation, called *Hartree approximation*, is to assume that the electrons as whole produce an average electrostatic energy potential V_{tot} , and that a given electron feels the resulting total potential

$$V_{tot} = U(x, y) - e\Phi(x, y, z) \quad . \quad (2)$$

The normed wave function satisfies the Schrödinger equation in the Effective Mass Approximation, i.e.

$$\left[E_c - \frac{\hbar^2}{2m^*} \Delta + V_{tot}(x, y, z) \right] \psi = E \psi \quad (3)$$

where E is the total energy, E_c the conduction band edge energy, and m^* denotes the effective mass of the electron in the conduction band. By inserting eq.(1) into eq.(3), in

each z -th cross section of the device, one obtains the following equation for the envelope function $\chi_{\alpha z}(x, y)$

$$\left[-\frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + U - e\Phi \right] \chi_{\alpha z} = \varepsilon_{\alpha z} \chi_{\alpha z} \quad , \quad E_{\alpha z} = \varepsilon_{\alpha z} + \frac{\hbar^2 k_z^2}{2m^*} + E_c \quad (4)$$

where $\varepsilon_{\alpha z}$ is the kinetic energy associated with the confinement in the x-y plane, and we have assumed parabolic band approximation. The term Φ satisfies the Poisson equation

$$\nabla \cdot [\epsilon \nabla \Phi(x, y, z)] = e(n - N_D + N_A) \quad (5)$$

where N_D, N_A are the doping profile (due to donors and acceptors) and $n(x, y, z, t)$ is the electron density, which depends on $\chi_{\alpha z}$

$$n(x, y, z, t) = \sum_{\alpha} \rho^{\alpha}(z, t) |\chi_{\alpha z}(x, y, t)|^2 \quad (6)$$

where ρ^{α} is the subband linear density in the z -direction

$$\rho^{\alpha}(z, t) = \frac{2}{2\pi} \int f_{\alpha}(z, k_z, t) dk_z \quad (7)$$

f_{α} being the electron distribution function in the α -subband. For an assigned confining potential, one has to solve a coupled problem formed by eqs.(4), (5) and (6) to find $\varepsilon_{\alpha z}, \chi_{\alpha z}$ in each cross-section.

The transport in the z -th direction is described using the MBTE [1]

$$\frac{\partial f_{\alpha}}{\partial t} + v_z(k_z) \frac{\partial f_{\alpha}}{\partial z} - \frac{e}{\hbar} \mathcal{E}_z \frac{\partial f_{\alpha}}{\partial k_z} = \sum_{\alpha'} \sum_{\eta} \mathcal{C}_{\eta}[f_{\alpha}, f_{\alpha'}] \quad (8)$$

where e is the absolute value of the electron charge, \hbar the Planck constant divided by 2π , and

$$v_z = \frac{1}{\hbar} \frac{\partial E_{\alpha z}}{\partial k_z} = \frac{\hbar k_z}{m^*} \quad , \quad \mathcal{E}_z = -\frac{1}{e} \frac{\partial E_{\alpha z}}{\partial z} \quad (9)$$

are respectively the electron group velocity and the electric field. In the low density approximation (not-degenerate case), the collisional operator writes

$$\mathcal{C}_{\eta}[f_{\alpha}, f_{\alpha'}] = \frac{L_z}{2\pi} \int dk'_z \{ w_{\eta}(\mathbf{k}', \mathbf{k}) f_{\alpha'}(k'_z) - w_{\eta}(\mathbf{k}, \mathbf{k}') f_{\alpha}(k_z) \} \quad (10)$$

where $w_{\eta}(\mathbf{k}, \mathbf{k}') = w_{\eta}(\alpha, k_z, \alpha', k'_z)$ is the η -th scattering rate. When $\alpha = \alpha'$ we have an intra-subband scattering, otherwise we have an inter-subband scattering.

Scattering mechanisms in SiNWs must comprise acoustic phonon scattering (bulk and confined), non-polar optical phonon scattering, surface scattering, scattering with ionized

impurities, as well as dielectric screening [4], [5]. However in this preliminary study, for the sake of simplicity, we shall limit ourselves to consider just scattering with optical and acoustic phonons. For the bulk acoustic phonon scattering, in the elastic equipartition approximation, the transition rate is given by [1]

$$w_{ac}(\mathbf{k}, \mathbf{k}') = s_{ac} G^{\alpha\alpha'} \delta(E_{\alpha'} - E_{\alpha}) \quad , \quad s_{ac} = \frac{2\pi D_A^2 k_B T_L}{\rho \hbar v_s^2 L_z} \quad (11)$$

where D_A is the acoustic deformation potential (9 eV), T_L the lattice temperature, ρ the mass density (2.33 gr/cm³), v_s the sound speed (6960 m/sec), and $G^{\alpha\alpha'}$ the confinement factor

$$G^{\alpha\alpha'} = \int |\chi_{\alpha'}(x, y)|^2 |\chi_{\alpha}(x, y)|^2 dx dy \quad . \quad (12)$$

For the optical phonons we have

$$w_{op}(\mathbf{k}, \mathbf{k}') = s_{op} \left[g_0 + \frac{1}{2} \mp \frac{1}{2} \right] G^{\alpha\alpha'} \delta(E_{\alpha'} - E_{\alpha} \mp \hbar\omega_0) \quad , \quad s_{op} = \frac{\pi D_0^2}{\rho \omega_0 L_z} \quad (13)$$

where D_0 is the optical deformation potential (11.4 10⁸ eV/cm), $\hbar\omega_0$ the effective optical phonon energy (63 meV), and g_0 the Bose-Einstein phonon occupation number.

3 Extended Hydrodynamic model

By multiplying the MBTE (8) by the weight functions $\psi_A = \{1, v_z, \varepsilon_z, v_z \varepsilon_z\}$, and integrating in the k_z space, one obtains the following hydrodynamic-like equations

$$\frac{\partial \rho^{\alpha}}{\partial t} + \frac{\partial(\rho^{\alpha} V^{\alpha})}{\partial z} = \rho^{\alpha} \sum_{\alpha'} C_{\rho}^{\alpha\alpha'} \quad (14)$$

$$\frac{\partial(\rho^{\alpha} V^{\alpha})}{\partial t} + \frac{2}{m^*} \frac{\partial(\rho^{\alpha} W^{\alpha})}{\partial z} + \frac{e}{m^*} \rho^{\alpha} \mathcal{E}_z = \rho^{\alpha} \sum_{\alpha'} C_V^{\alpha\alpha'} \quad (15)$$

$$\frac{\partial(\rho^{\alpha} W^{\alpha})}{\partial t} + \frac{\partial(\rho^{\alpha} S^{\alpha})}{\partial z} + \rho^{\alpha} e \mathcal{E}_z V^{\alpha} = \rho^{\alpha} \sum_{\alpha'} C_W^{\alpha\alpha'} \quad (16)$$

$$\frac{\partial(\rho^{\alpha} S^{\alpha})}{\partial t} + \frac{\partial(\rho^{\alpha} F^{\alpha})}{\partial z} + 3 \frac{e}{m^*} \rho^{\alpha} \mathcal{E}_z W^{\alpha} = \rho^{\alpha} \sum_{\alpha'} C_S^{\alpha\alpha'} \quad (17)$$

in the unknowns (called moments)

$$V^{\alpha} = \frac{2}{(2\pi)} \frac{1}{\rho^{\alpha}} \int_{\mathbb{R}} f_{\alpha}(z, k_z, t) v_z dk_z \quad (\text{subband velocity}), \quad (18)$$

$$W^{\alpha} = \frac{2}{(2\pi)} \frac{1}{\rho^{\alpha}} \int_{\mathbb{R}} f_{\alpha}(z, k_z, t) \varepsilon_z dk_z \quad (\text{subband energy}), \quad (19)$$

$$S^{\alpha} = \frac{2}{(2\pi)} \frac{1}{\rho^{\alpha}} \int_{\mathbb{R}} f_{\alpha}(z, k_z, t) \varepsilon_z v_z dk_z \quad (\text{subband energy- flux}) \quad (20)$$

and the higher-order flux F^α , and the production terms

$$F^\alpha = \frac{2}{(2\pi)} \frac{1}{\rho^\alpha} \int f_\alpha v_z^2 \varepsilon_z dk_z \quad (21)$$

$$C_\rho^{\alpha\alpha'} = \frac{2}{(2\pi)} \frac{1}{\rho^\alpha} \sum_\eta \int \mathcal{C}_\eta[f_\alpha, f_{\alpha'}] dk_z \quad (22)$$

$$C_V^{\alpha\alpha'} = \frac{2}{(2\pi)} \frac{1}{\rho^\alpha} \sum_\eta \int \mathcal{C}_\eta[f_\alpha, f_{\alpha'}] v_z dk_z \quad (23)$$

$$C_W^{\alpha\alpha'} = \frac{2}{(2\pi)} \frac{1}{\rho^\alpha} \sum_\eta \int \mathcal{C}_\eta[f_\alpha, f_{\alpha'}] \varepsilon_z dk_z \quad (24)$$

$$C_S^{\alpha\alpha'} = \frac{2}{(2\pi)} \frac{1}{\rho^\alpha} \sum_\eta \int \mathcal{C}_\eta[f_\alpha, f_{\alpha'}] \varepsilon_z v_z dk_z \quad (25)$$

This system of PDEs is of hyperbolic type and it is not closed, i.e. there are more unknowns than equations. The Maximum Entropy Principle leads to a systematic way for obtaining constitutive relations on the basis of the information theory [14], as already proved successfully in the bulk case [15]-[19], and for quantum well structures [20], [21]. Actually, in a semiconductor electrons interact with phonons describing the thermal vibrations of the ions placed at the points of the crystal lattice. However, since we are considering the phonon gas as a thermal bath, one has to extremize only the electron component of the entropy. We define the entropy of the electronic system as

$$S_e = \sum_\alpha |\chi_\alpha(x, y, t)|^2 S_e^\alpha \quad (26)$$

$$S_e^\alpha = -\frac{2}{(2\pi)} k_B \int_{\mathbb{R}} (f_\alpha \log f_\alpha - f_\alpha) dk_z \quad , \quad (27)$$

and, according to MEP, we estimate the f_α 's as the distributions that maximize S_e under the constraints that the basic moments, which we have previously considered, are assigned. In a neighborhood of local thermal equilibrium, this distribution function writes [22]

$$\hat{f}_\alpha = \exp\left(-\frac{\lambda^\alpha}{k_B} - \lambda_W^\alpha \varepsilon_z\right) \left\{1 - \tau \left(\hat{\lambda}_V^\alpha v_z + \hat{\lambda}_S^\alpha v_z \varepsilon_z\right)\right\} \quad (28)$$

where the quantities $(\lambda^\alpha, \lambda_W^\alpha, \hat{\lambda}_V^\alpha, \hat{\lambda}_S^\alpha)$ are known functions of the moments $\{\rho^\alpha, V^\alpha, W^\alpha, S^\alpha\}$. By using the distribution function (28) it is possible to evaluate the unknown functions appearing in the balance equations by integration. In this way the higher-order flux term writes

$$F^\alpha = \frac{6(W^\alpha)^2}{m^*} \quad (29)$$

as well as the production terms $C_\rho^{\alpha\alpha'}$, $C_V^{\alpha\alpha'}$, $C_W^{\alpha\alpha'}$, $C_S^{\alpha\alpha'}$ have been determined. We want underline that this Extended Hydrodynamic model has been closed by using first principles, and it is free of any fitting parameters.

4 Electron Mobility

The mobility is one of the most important parameters that determine the performance of a field-effect transistor. At low electric field, the carrier drift velocity is proportional to the electric field strength, and the proportionality constant is defined as the mobility. Hence a higher mobility material is likely to have higher frequency response, because carriers take less time to travel through the device. When the fields are sufficiently large, nonlinearities in the mobility and saturation in the drift velocity are observed. In fact, the scattering of the carriers with the lattice, the impurities, and the surface is more active for higher fields, and the charges lose the energy gained by the electric field.

Now we want to prove that our Extended Hydrodynamic model is able to predict such behaviours. We shall assume that the wire is surrounded by an oxide which gives rise to an infinitely deep potential barrier. In such a case, the following analytical relations for the bottom energies and envelope functions can be used [1]

$$\varepsilon_\alpha = \frac{\hbar^2 \pi^2}{2m^*} \left(\frac{n^2}{L_x^2} + \frac{m^2}{L_y^2} \right) \quad , \quad \chi_\alpha = \sqrt{\frac{2}{L_x}} \sin \left(\frac{n\pi}{L_x} x \right) \sqrt{\frac{2}{L_y}} \sin \left(\frac{m\pi}{L_y} y \right) \quad n, m \in \mathbb{N}. \quad (30)$$

To obtain the drift velocity and the mobility, we have performed a numerical integration of our hydrodynamic model in the stationary homogeneous case with a constant electric field along the z direction. In this case the unknowns ($\rho^\alpha, V^\alpha, W^\alpha, S^\alpha$) depend on the time only. The initial data are the equilibrium values, obtained with a global maxwellian with lattice temperature T_0 (300 K), i.e.

$$V^\alpha(0) = 0 \quad , \quad W^\alpha(0) = \frac{1}{2} k_B T_0 \quad , \quad S^\alpha(0) = 0 \quad (31)$$

$$\rho^\alpha(0) = L_x L_y N_D \frac{\exp \left(-\frac{\varepsilon_\alpha}{k_B T_0} \right)}{\sum_\alpha \exp \left(-\frac{\varepsilon_\alpha}{k_B T_0} \right)} \quad , \quad (32)$$

where N_D is the number of donor impurities. The average drift velocity is defined as

$$\langle V \rangle = \frac{\sum_\alpha \rho^\alpha V^\alpha}{\sum_\alpha \rho^\alpha} \quad . \quad (33)$$

In the figure 1 we plot the subband velocities V^α ($\alpha = 1, \dots, 4$) as well as the average drift velocity versus the simulation time, for an electric field of 1000 V/cm, with $L_x = L_y = 10$ nm. The stationary regime is reached in a few picoseconds, and the typical phenomenon of saturation is qualitatively and quantitatively well described.

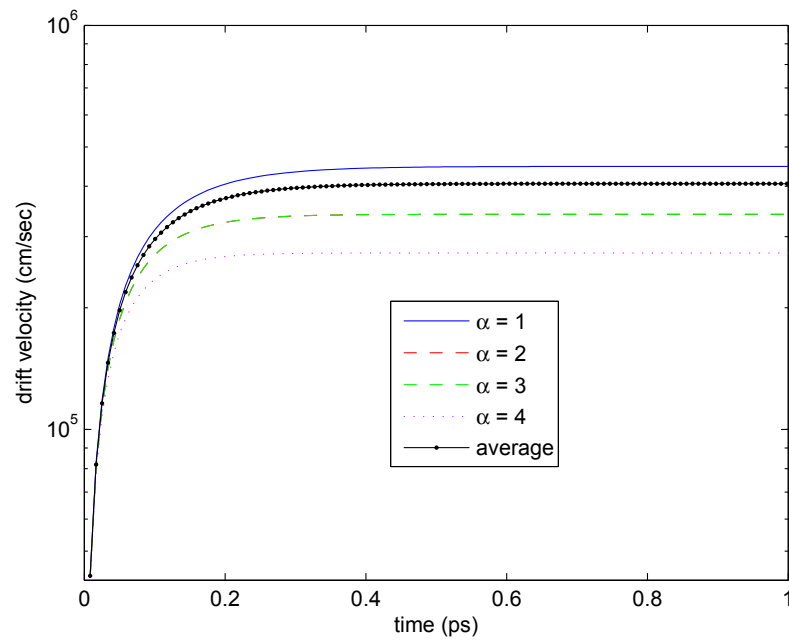


Figure 1: The subband drift velocities V^α and the average drift velocity (33) versus the simulation time, for an electric field of 1000 V/cm, with $L_x = L_y = 10$ nm.

In the figure 2 we plot the average drift velocity, obtained in the stationary regime, versus the electric field from which we can evaluate the saturation velocity $v_s = 6.7 \cdot 10^6$ cm/sec.

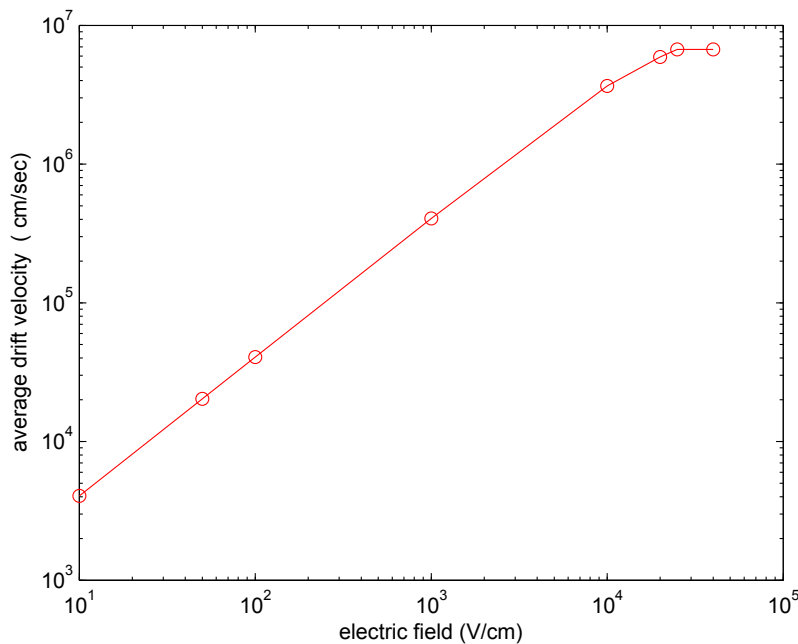


Figure 2: The average drift velocity (33), obtained in the stationary regime, versus the electric field with $L_x = L_y = 10$ nm.

The average mobility is

$$\mu = \frac{\sum_{\alpha} \rho^{\alpha} \mu^{\alpha}}{\sum_{\alpha} \rho^{\alpha}} \quad , \quad \mu^{\alpha} = \frac{V^{\alpha}}{\mathcal{E}_z} \quad (34)$$

where μ^{α} is the subband mobility. In the figure 3 we plot the average mobility as function of the electric field. We notice for low fields (≤ 1000 V/cm) the mobility is constant (i.e. $\mu_0 = 406$ cm² V/sec) whereas, for high fields, the mobility decreases because the scattering processes become more active. In the latter figure for comparison we have also reported the mobility given by the Caughey-Thomas formula [23]

$$\mu_C = \mu_0 \left[1 + \left(\frac{\mu_0 \mathcal{E}_z}{v_s} \right)^2 \right]^{-\frac{1}{2}} \quad . \quad (35)$$

Similar results have been obtained using MC simulations [4], but with more expensive computational times.

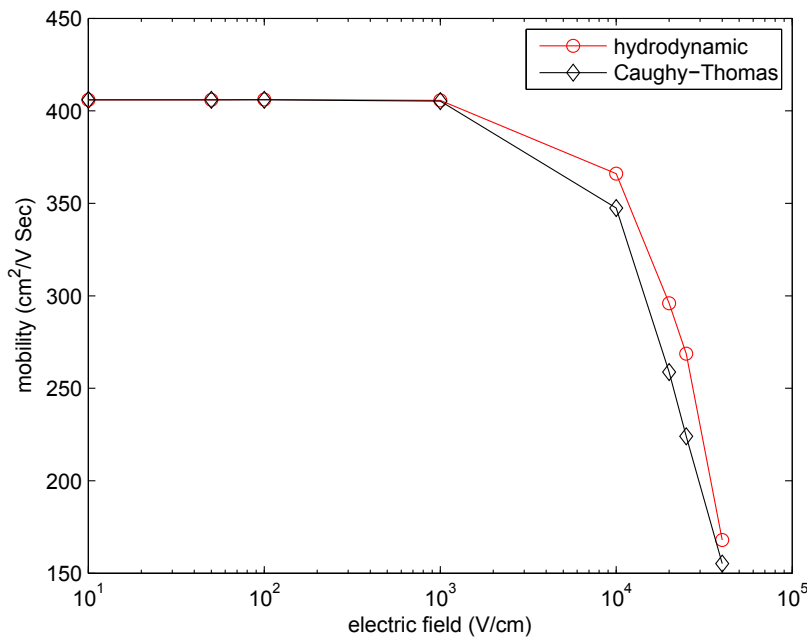


Figure 3: The average mobility $(34)_1$ (circles) versus the electric field with $L_x = L_y = 10$ nm, and the mobility evaluated using the Caughey-Thomas formula (diamonds).

5 Conclusions

An extended hydrodynamic model for SiNWs has been formulated with the use of the maximum entropy principle, where the transport coefficients are completely determined without any fitting procedure. Using this model we have evaluated the electron mobility (low and high-field), which is in agreement with MC simulation results. However, our model must be improved by including other relevant scattering mechanisms such as scattering with impurities, surface roughness, acoustic confined phonons. Simulation of real device as well as the study of thermoelectric effects according to the guideline in [24]-[28] are under investigation, and they will be published in the next future.

Acknowledgment

We acknowledge the support of the Università degli Studi di Catania, MIUR PRIN 2009 "Problemi Matematici delle Teorie Cinetiche e Applicazioni", and the CINECA Award N. HP10COORUX 2012.

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