IW²

BOOKLET

1st International Wigner Workshop

November 29, 2015
Waikoloa, Hawaii, USA

In conjunction with
ISANN 2015
International Symposium on
Advanced Nanodevices and Nanotechnology
November 29-December 4, 2015
Waikoloa, Hawaii, USA

organized by
Wigner Initiative

Preface

Aloha!

We would like to welcome you to Hawaii and to the 1^{st} International Wigner Workshop (IW2), which is hosted by the 2015 International Symposium on Advanced Nanodevices and Nanotechnology. The workshop is being held on Sunday, November 29 in the *Waters Edge Boardroom* of the *Hilton Waikoloa Village Hotel* and is organized by the Wigner Initiative. This workshop brings together researchers to foster discussion on the current state and future directions of Wigner-related research. The workshop is composed of three overview talks, each introducing a specific topic. The overview talks are complemented by five short talks to present some data. The submitted abstracts were reviewed by the workshop chairs and the program committee.

This booklet contains the scientific program, the abstracts accepted for presentation, as well as an overview of the special issue on Wigner functions, published in the Journal of Computational Electronics.

We would like to express our gratitude to the participants to support our workshop and we hope that you enjoy it as well as the host conference and your stay in Hawaii.

David K. Ferry and Josef Weinbub
Chairs of IW2 2015
November 22, 2015

Workshop Chairs

David K. Ferry	Arizona State University, USA
Josef Weinbub	TU Wien, Austria

Program Committee

Irena Knezevic	University of Wisconsin-Madison, USA
Mihail Nedjalkov	TU Wien, Austria and Bulgarian Academy of Sciences, Bulgaria
Siegfried Selberherr	TU Wien, Austria

Speakers

Wei Cai	University of North Carolina at Charlotte, USA
David K. Ferry	Arizona State University, USA
Kyoung-Youm Kim	Sejong University, Korea
Bartlomiej J. Spisak	AGH University of Science and Technology, Poland
Zhangpeng Sun	Peking University, China
Ting-wei Tang	University of Massachusetts, USA
Josef Weinbub	TU Wien, Austria

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1 Program

Location: Waters Edge Boardroom - Chair: Josef Weinbub

Each talk slot contains five minutes of Q&A!

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D.K. Ferry
Wigner Functions, Variations and Entanglement

09:30-09:50 (Short Talk)
B.J. Spisak, M. Wołoszyn
Wigner Representation of Electron Dynamics in Presence of Thermal Dephasing in Disordered Systems

09:50-10:10 (Short Talk)
K.-Y. Kim, S. Kim
Uncertainty and Quantum Correlation in Discrete Wigner Transport Equations

SESSION II - Boundary Conditions

10:10-10:40 (Overview Talk)
J.-H. Lee, M. Shin, T. Tang
Review of Boundary Conditions and Discretization Schemes for the Solution of Wigner Transport Equation

10:40-11:00 (Short Talk)
A. Arnold, R. Li, T. Lu, Z. Sun
Convergence of Stationary Wigner Equation with Inflow Boundary Conditions

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SESSION III - Simulations and Applications

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Adaptive Conservative Chebyshev Polynomial Spectral Element Methods for Transient Wigner Equation in Quantum Transport

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ViennaWD - Status and Outlook

12:35-12:55 (Short Talk)
P. Ellinghaus, J. Weinbub, M. Nedjalkov, S. Selberherr
ViennaWD - Applications

2 Abstracts

2.1 Wigner Functions, Variations and Entanglement

D.K. Ferry
Arizona State University, USA
ferry@asu.edu

I will discuss the formulation of the Wigner function, and various other phase space functions that have been used in the literature. I will discuss the limitations of these alternative forms. Then I will talk about entanglement that can exist in the Wigner form for multiple particles, and how it can be used in other applications.

2.2 Wigner Representation of Electron Dynamics in Presence of Thermal Dephasing in Disordered Systems

B.J. Spisak, M. Wołoszyn
AGH University of Science and Technology, Poland
bjs@agh.edu.pl

Electron transport phenomena in disordered systems demonstrate the non-Markovian properties due the quantum interference of the conduction electrons in the absence of mechanisms which destroy the time-reversal invariance. One of the possible manifestations of the quantum interference in the disordered systems is the weak localization of the carriers. The effect stems from the coherent propagation of the electrons which are multiply scattered on the spatially distributed ions.

In the present contribution, an influence of an effective thermal field due to the dynamics of ions on the weak localization is considered in terms of the generalized kinetic equation in the Wigner representation. Within this approach, the weak localization manifests itself by the singularity for the multiple backward scattering of the carriers, and we show that this singularity is removed by the considered dephasing mechanism.

2.3 Uncertainty and Quantum Correlation in Discrete Wigner Transport Equations

K.-Y. Kim[1], S. Kim[2]
[1]Sejong University, Korea
[2]Hankuk University of Foreign Studies, Korea
kykim@sejong.ac.kr

In this presentation, we discuss two fundamental characteristics of the discrete Wigner transport equation resulting from the uncertainty principle. First, the discretized momentum space results in a kind of positional uncertainty of electrons. We show that this uncertainty determines the maximum length of nonlocal potential correlation. As a result, the finer the momentum resolution of the discrete Wigner function is, the longer the region for nonlocal potential correlation becomes. Next, electrons can have positional uncertainty inside the device. We prove that this uncertainty sets a minimum momentum resolution of the discrete Wigner function to be h/(2L), where h and L denote the Planck constant and the length of the device, respectively. Therefore, the smaller the device is, the larger the minimum momentum resolution should be. We show numerically that its violation deteriorates the simulation results significantly.

2.4 Review of Boundary Conditions and Discretization Schemes for the Solution of Wigner Transport Equation

J.-H. Lee[1], M. Shin[1], T. Tang[2]
[1]KAIST, Korea
[2]University of Massachusetts, USA
ttang@ecs.umass.edu

We review the conventional boundary conditions (BCs) and discretization schemes used for the solution of Wigner transport equation (WTE). The most often used BC is Frensleys U-scheme [1] with the equilibrium Fermi-Dirac distribution function (F-D DF). The other is the drifted F-D DF by adjusting the drift k-vector iteratively to maintain the current continuity [2,3] and/or the charge neutrality [4]. To take the reservoir-device interaction (R-D I) into consideration, Ho and Yamaguchi [5] moved the artificial boundaries inside the reservoir. Knezevic [3] treated the R-D I via Markovian hopping model. Dolcini et al. [6] used a relaxation-time-approximation model for energy dissipation due to the R-D I. For finite differencing schemes used in approximating the kinetic term of WTE, the simplest one is the up/downwind first-order differencing scheme (FDS) [1]. The second-order differencing scheme (SDS) was used by Jensen and Buot [7] which necessitates introduction of additional contact grids. The differencing schemes (DSs) of higher orders were used by Kim and Lee [8]. Recently, Yamada et al. [9] have used a third-order differencing scheme (TDS) which can be viewed as a combination of central differencing scheme (CDS) and SDS. Comparison of simulation results for a ballistic gate-all-around nanowire transistor using different BCs and DSs will be presented.

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[7] K. L. Jensen and F. A. Buot, IEEE Trans. Elec. Dev. 38, 2337 (1991).
[8] K.-Y. Kim and B. Lee, Sol.-St. Elec. 43, 2243 (1999).
[9] Y. Yamada, H. Tsuchiya, and M. Ogawa, IEEE Trans. Elec. Dev. 56, 1396 (2009).

2.5 Convergence of Stationary Wigner Equation with Inflow Boundary Conditions

A. Arnold[1], R. Li[2], T. Lu[2], Z. Sun[2]
[1]TU Wien, Austria
[2]Peking University, China
sunzhangpeng@pku.edu.cn

We propose in this paper a well-posed semi-discretization of the stationary Wigner equation with inflow BCs, making use of the Whittaker-Shannon interpolation formula with shifted sampling points. The convergence of the solutions of the discrete problem to the continuous problem is then analyzed, providing certain regularity of the solution of the continuous problem.

2.6 Adaptive Conservative Chebyshev Polynomial Spectral Element Methods for Transient Wigner Equation in Quantum Transport

W. Cai
University of North Carolina at Charlotte, USA
wcai@uncc.edu

We will present a cell average spectral element method (SEM) for solving the time-dependent Wigner equation for transport in quantum devices. The cell average SEM with Chebyshev orthogonal polynomials in the phase space has two distinct features: (1) no artificial periodic boundary conditions in the k-space as in Fourier series based approximations, (2) allowing adaptive non-uniform meshes to reduce the high-dimensional computational cost of Wigner functions while preserving exactly the mass conservation for the numerical solutions. This conservation property is a result of the use of k-cell averages of the Wigner distribution and their exact analytical transformation to and from the Wignerdistribution function itself. Numerical results with the method are provided to demonstrate its high accuracy, conservation, convergence and a reduction of the cost using adaptive meshes.

Reference:

[1] Sihong Shao, Tiao Lu and Wei Cai, Adaptive Conservative Cell Average Spectral Element Methods for Transient Wigner Equation in Quantum Transport, Communications in Computational Physics, Vol. 9, No. 3, pp. 711-739, March 2011.

2.7 ViennaWD - Status and Outlook

J. Weinbub[1], P. Ellinghaus[1], M. Nedjalkov[1,2], S. Selberherr[1]
[1]TU Wien, Austria
[2]Bulgarian Academy of Sciences, Bulgaria
weinbub@iue.tuwien.ac.at

We will present the current state of the Wigner Monte Carlo quantum transport simulator shipped with the free open source software package ViennaWD. The underlying Wigner transport model based on signed particles will be briefly introduced and compared to the alternative affinity approach. The applied spatial domain decomposition-based parallelization approach, which drastically reduces simulation time, is discussed. Additional simulator features, such as usability and supported output quantities, will be described. The future road map will be laid out, focusing on self-consistency, load-balanced parallelization approaches, and the use of modern large-scale computing platforms. The current computational and numerical challenges will be presented. A discussion regarding missing features or feature prioritization will be triggered to tune the future research and Wigner model development road map.

2.8 ViennaWD - Applications

P. Ellinghaus[1], J. Weinbub[1], M. Nedjalkov[1,2], S. Selberherr[1]
[1]TU Wien, Austria
[2]Bulgarian Academy of Sciences, Bulgaria
weinbub@iue.tuwien.ac.at

The Wigner Monte Carlo simulator - part of the free open source ViennaWD project - implements the signed-particle method, which has been matured to the point where two-dimensional numerical experiments can be performed accurately and with a reasonable computational effort. The capability of the Wigner simulator to investigate time-dependent quantum transport is demonstrated by examples investigating the evolution of wave packets. The propagation of a wave packet in a mesoscopic ring-like structure reveals the quantum phenomena of interference and also entanglement, which can be clearly identified using the phase-space perspective. Furthermore, the use of electrostatic lenses to manipulate electron wave packets will be discussed along with a demonstration on how focusing can be used to increase the drive-current in nanoscale channels. An outline of envisioned simulation experiments, which consider decoherence effects and magnetic fields, will be given to highlight the associated theoretical and computational challenges for the Wigner signed-particle model.

3 Overview of Special Issue on Wigner Functions

Journal of Computational Electronics

Closely related to this workshop is the recently published Special Issue on Wigner Functions in the Journal of Computational Electronics, which was edited by M. Nedjalkov, J. Weinbub, and D.K. Ferry. This Chapter gives an overview of the contributions published in this special issue, by providing the publication information as well as the individual abstracts.

3.1 Introduction to the Special Issue on Wigner Functions

M. Nedjalkov[1,2], J. Weinbub[1], D.K. Ferry[3]
[1]TU Wien, Austria
[2]Bulgarian Academy of Sciences, Bulgaria
[3]Arizona State University, USA
nedjalkov@iue.tuwien.ac.at
Journal of Computational Electronics **14**(4), pp.857-858, 2015.
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The Wigner function was first derived by E.P. Wigner around 1931 as an exotic outcome of the wave mechanics which, being defined in the phase space, does not favor either coordinate or momentum variables. Pioneered by H.J. Groenewold and J.E. Moyal the Wigner formulation of quantum mechanics evolved until the end of last century, to a fully autonomous, independent alternative to Hilbert space mechanics and path integral formulations. As S. MacLane put it *(Ladies and) gentlemen: There is lots of room left in Hilbert Space*, the same holds true for the phase space, where Wigner and alternative approaches, like Husimi and Bohmian distributions, are easily accommodated.

Applied to challenges in computational electronics, the Wigner approach offers the unique ability to describe transient problems for open systems by simultaneously accounting for different levels of approximation for the effects of the degrees of freedom associated with the environment. For example, the WignerBoltzmann equation enables the formalism with the efficient Boltzmann model of collisions (local in position/time) with phonons and impurities featuring the classical era of microelectronics. The equation bridges the gap between classical and quantum electron dynamics, ensuring a seamless transition between coherent and scattering dominated modes of transport. This approach has been applied to simulate stationary and transient behavior of nanostructures, superlattices, to investigate processes of decoherence, quantum chaos, and recently beyond transport tasks in density functional theory and many body effects. The continuous accumulation of knowledge results in increased publication activities.

A good example is the fact that two books by C. Jacoboni as well as D. Querlioz and P. Dollfus have been published in the year 2010, summarizing the theoretical and applied achievements of the Wigner research. Nevertheless, critics claim that, although various groups pick up the work, they abandon it again, never delivering a compelling research result. This criticism has been addressed by the Wigner community with the founding of the Wigner Initiative[1] in 2015, bringing all research in this area closer together, thereby increasing synergy effects and fostering knowledge transfer.

This special issue is the first effort of the Initiative in this direction and comprises theoretical analysis, numerical aspects, and recent applications of the Wigner formalism, as well as comparisons with alternative phase space quasi-distribution functions and other quantum-mechanical approaches. In contrast to books, the purpose of which is to provide a systematic description, the contributions in this special issue rather highlight selected achievements in the field along with important logical and philosophical points in the phase space formulations of quantum mechanics. In particular, this special issue contains nine contributions characterized in the following:

I. Dimov et al. investigate the role of boundary conditions for the existence and the uniqueness of the solution of the stationary and transient formulations of the Wigner equation.

D.K. Ferry provides an overview of different phase-space approaches with a special focus on quantum properties, such as entanglement, complemented by identifying core strengths of the Wigner approach.

B.J. Hiley discusses the close relationship between the Wigner-Moyal algebra and the original noncommutative quantum algebra introduced by von Neumann.

O. Jonasson et al. employ the Wigner function formalism to simulate partially coherent, dissipative electron transport in biased semiconductor superlattices, underlining the practical capabilities of Wigner function approaches.

M. Nedjalkov et al. introduce an analysis of formulations of the Wigner equation under a general gauge for the electric field, striving to develop alternative computational methods applied in the Wigner formalism.

E. Coloms et al. compare the Wigner, Husimi, and Bohmian distributions with respect to constructing a well-defined phase space distribution, providing a critical view on the properties of the individual formulations.

J.M. Sellier et al. analyzed a harmonic oscillator from the Wigner perspective. A brief review on utilizing a phase-space approach is given as well as the feasibility of the so-called signed particle Monte Carlo method is shown.

B.J. Spisak et al. apply the Wigner function to the description of the dynamics of conduction electrons in finite one-dimensional systems with randomly distributed scattering centers.

J. Weinbub et al. investigate parallelization strategies for two-dimensional Wigner Monte Carlo method based on the signed particle approach, enabling to utilize large-scale computing resources to stem the significant memory and computing demands.

As the guest editors of this special issue we would like to thank all authors for their contributions.

[1] http://www.iue.tuwien.ac.at/wigner-wiki/.

3.2 Boundary Conditions and the Wigner Equation Solution

I.Dimov[1], M. Nedjalkov[1,2], J.M. Sellier[1], S. Selberherr[2]
[1]Bulgarian Academy of Sciences, Bulgaria
[2]TU Wien, Austria
ivdimov@bas.bg
Journal of Computational Electronics **14**(4), pp.859-863, 2015.
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We consider the existence and uniqueness of the solution of the Wigner equation in the presence of boundary conditions. The equation, describing electron transport in nanostructures, is analyzed in terms of the Neumann series expansion of the corresponding integral form, obtained with the help of classical particle trajectories. It is shown that the mathematical aspects of the solution can not be separated from the physical attributes of the problem. In the presented analysis these two sides of the problem mutually interplay, which is of importance for understanding of the peculiarities of Wigner-quantum transport. The problem is first formulated as the long time limit of a general evolution process posed by initial and boundary conditions. Then the Wigner equation is reformulated as a second kind of a Fredholm integral equation which is of Volterra type with respect to the time variable. The analysis of the convergence of the corresponding Neumann series, sometimes called LiouvilleNeumann series, relies on the assumption for reasonable local conditions obeyed by the kernel.

3.3 Phase-Space Functions: Can They Give a Different View of Quantum Mechanics?

D.K. Ferry
Arizona State University, USA
ferry@asu.edu
Journal of Computational Electronics **14**(4), pp.864-868, 2015.
doi:10.1007/s10825-015-0731-z

The Wigner function has been studied for more than eight decades, in the quest to develop a phase-space formulation of quantum mechanics. But, it is not the only phase-space formulation. Here, we discuss the properties of some of the various phase-space approaches and how they can give new insights into many quantum properties such as entanglement, which is not normally observable.

3.4 On the Relationship Between the Wigner-Moyal Approach and the Quantum Operator Algebra of von Neumann

B.J. Hiley[1,2]
[1]University College London, UK
[2]University of London, UK
b.hiley@bbk.ac.uk
Journal of Computational Electronics **14**(4), pp.869-878, 2015.
doi:10.1007/s10825-015-0728-7

In this paper we discuss the close relationship between the WignerMoyal algebra and the original non-commutative quantum algebra introduced by von Neumann in 1931. We show that the ”distribution function”, F(P, X, t) is simply the quantum mechanical density matrix for a single particle where the coordinates, X and P, are not the coordinates of a point particle, but the mean co-ordinate of a cell structure (a ’blob’) in phase space. This provides an intrinsically non-local and non-commutative description of an individual, which only becomes a point particle in the commutative limit. In this general structure, the Wigner function appears as a transition probability amplitude which accounts for the appearance of negative values. The Moyal and Baker brackets play a significant role in the time evolution, producing the quantum HamiltonJacobi equation used in the Bohm approach. It is the non-commutative structure based on a symplectic geometry that generates a generalised phase space for quantum processes.

3.5 Dissipative Transport in Superlattices Within the Wigner Function Formalism

O. Jonasson, I. Knezevic
University of Wisconsin at Madison, USA
ojonasson@wisc.edu
Journal of Computational Electronics **14**(4), pp.879-887, 2015.
doi:10.1007/s10825-015-0734-9

We employ the Wigner function formalism to simulate partially coherent, dissipative electron transport in biased semiconductor superlattices. We introduce a model collision integral with terms that describe energy dissipation, momentum relaxation, and the decay of spatial coherences (localization). Based on a particle-based solution to the Wigner transport equation with the model collision integral, we simulate quantum electronic transport at 10 K in a GaAs/AlGaAs superlattice and accurately reproduce its current density vs field characteristics obtained in experiment.

3.6 The Wigner Equation in the Presence of Electromagnetic Potentials

M. Nedjalkov[1,2], J. Weinbub[2], P. Ellinghaus[2], S. Selberherr[2]
[1]Bulgarian Academy of Sciences, Bulgaria
[2]TU Wien, Austria
nedjalkov@iue.tuwien.ac.at
Journal of Computational Electronics **14**(4), pp.888-893, 2015.
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An analysis of the possible formulations of the Wigner equation under a general gauge for the electric field is presented with an emphasis on the computational aspects of the problem. The numerical peculiarities of those formulations enable alternative computational strategies based on existing numerical methods applied in the Wigner formalism, such as finite difference or stochastic particle methods. The phase space formulation of the problem along with certain relations to classical mechanics offers an insight about the role of the gauge transforms in quantum mechanics.

3.7 Comparing Wigner, Husimi and Bohmian Distributions: Which One is a True Probability Distribution in Phase Space?

E. Colomés, Z. Zhan, X. Oriols
Universitat Autònoma de Barcelona, Spain
xavier.oriols@uab.es
Journal of Computational Electronics **14**(4), pp.894-906, 2015.
doi:10.1007/s10825-015-0737-6

The Wigner distribution function is a quasi-probability distribution. When properly integrated, it provides the correct charge and current densities, but it gives negative probabilities in some points and regions of the phase space. Alternatively, the Husimi distribution function is positive-defined everywhere, but it does not provide the correct charge and current densities. The origin of all these difficulties is the attempt to construct a phase space within a quantum theory that does not allow well-defined (i.e. simultaneous) values of the position and momentum of an electron. In contrast, within the (de Broglie-Bohm) Bohmian theory of quantum mechanics, an electron has well-defined position and momentum. Therefore, such theory provides a natural definition of the phase space probability distribution and by construction, it is positive-defined and it exactly reproduces the charge and current densities. The Bohmian distribution function has many potentialities for quantum problems, in general, and for quantum transport, in particular, that remains unexplored.

3.8 Wigner Functions, Signed Particles, and the Harmonic Oscillator

J.M. Sellier, I. Dimov
Bulgarian Academy of Sciences, Bulgaria
jeanmichel.sellier@parallel.bas.bg
Journal of Computational Electronics **14**(4), pp.907-915, 2015.
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In this paper, we introduce the simple harmonic oscillator and we address it in the Wigner formulation of quantum mechanics, therefore describing the whole problem in terms of quasi-distribution functions defined over the phase-space. The harmonic oscillator represents a very important problem as it provides exact solutions in both stationary and transient regimes. Subsequently, we outline the time-dependent signed particle Wigner Monte Carlo method and simulate the oscillator problem starting from stationary initial conditions, i.e. rotationally invariant functions in the phase-space, showing no evolution in time of the distribution function as expected. This work is, thus, twofold. On the one hand, one may see it as a short review effort to demonstrate the convenience of utilizing a phase-space approach in this particular context, suggesting that it could be the case again for different interesting problems. On the other hand, it represents a further opportunity to validate the signed particle Monte Carlo method, showing that a new reliable and powerful tool is available for the time-dependent simulation of quantum systems.

3.9 Dynamical Localisation of Conduction Electrons in One-Dimensional Disordered Systems

B.J. Spisak, M. Wołoszyn, D. Szydłowski
AGH University of Science and Technology, Poland
bjs@agh.edu.pl
Journal of Computational Electronics **14**(4), pp.916-921, 2015.
doi:10.1007/s10825-015-0733-x

The phase-space approach based on the Wigner distribution function is applied to the description of dynamics of conduction electrons in finite one-dimensional systems with randomly distributed scattering centres. It is shown that the coherent multiple scattering of the carriers in the disordered environment leads to the slowdown of its dynamics due to the weak localisation. This quantum phenomenon can be treated as a source of the subdiffusion of the quantum particles.

3.10 Domain Decomposition Strategies for the Two-Dimensional Wigner Monte Carlo Method

J. Weinbub[1], P. Ellinghaus[1], M. Nedjalkov[1,2]
[1]TU Wien, Austria
[2]Bulgarian Academy of Sciences, Bulgaria
weinbub@iue.tuwien.ac.at
Journal of Computational Electronics **14**(4), pp.922-929, 2015.
doi:10.1007/s10825-015-0730-0

A domain decomposition approach for the parallelization of the Wigner Monte Carlo method allows the huge memory requirements to be distributed amongst many computational units, thereby making large multi-dimensional simulations feasible. Two domain decomposition techniques-a uniform slab and uniform block decomposition-are compared and the design and implementation of the block decomposition approach, using the message passing interface, is discussed. The parallel performance of the two approaches is evaluated by simulating a representative physical problem. Our results show that the presumably inferior slab decomposition method is in fact superior to the block decomposition approach, due to the additional overhead incurred by the block decomposition method to set up its communication layer.