

3rd International Wigner Workshop

IW² 2019

Book of Abstracts

May 19-20, 2019

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Edited by

**David K. Ferry
Josef Weinbub
Stephen Goodnick**

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Welcome to the **Third International Wigner Workshop (IW²)**. The workshop is a two day meeting and brings together researchers from all areas of science and engineering areas in which Wigner functions have been or could be applied. The 2019 Workshop marks the third instalment of this series (the first and second were held in Hawaii, USA, in December 2015 and in the Lake District, UK, in June 2017) and further fosters the growing Wigner community (www.iue.tuwien.ac.at/wigner-wiki/). The speakers at this year's workshop provided an abstract which was reviewed by the program committee. Topics of interest are (but not limited to): Computational or Numerical Challenges, Nanoelectronics, Nanostructures, Quantum Circuits, Quantum Information Processing, Quantum Optics, Quantum Physics, and Quantum Transport. The workshop hosts four invited speakers and accepted seventeen regular speakers.

We would like to express our gratitude to our sponsors (in particular the SFB 767, Controlled Nanosystems, University of Konstanz – Prof. Wolfgang Belzig) as well as the participants who will make the workshop both interesting and successful. We hope that you enjoy it, as well as the host conference, and your stay in Evanston, IL.

*David K. Ferry, Josef Weinbub, and Stephen Goodnick
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Program

Sunday, May 19

8:00 am *Registration*

8:50 **Opening Remarks:** Josef Weinbub

9:00 **Session 1: Quantum Statistics**

Chair: David K. Ferry

9:00 Mark Everitt, *Loughborough University, UK*, “Quantum Mechanics of Anything (From Qubits to Atoms and Molecules) as a Statistical Theory (i.e. in Phase Space)” (Invited) 1

9:45 *General questions and discussion*

10:00 Lindsay Orr¹, Lisandro Hernandez de la Pena², and Pierre-Nicholas Roy¹, ¹*University of Waterloo, Canada*, ²*Kettering University, USA*, “Microcanonical Centroid Framework and the Wigner Distribution”

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10:20 *Coffee break*

10:50 Bartłomiej J. Spisak and Maciej Wołoszyn, *AGH University of Science and Technology, Poland*, “Dynamics of the Wigner Distribution Function on the Bunimovich Stadium” 4

11:10 **Session 2: Plasmas and Optics**

Chair: Josef Weinbub

11:10 Gert Brodiin, Robin Ekman, and Jens Zamanian, *Umea University, Sweden*, “Non-Linear Damping due to Multi-Plasmon Resonances”

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11:30 Gert Brodin, Jens Zamanian, Robin Ekman, and Haider Al-Naseri, *Umea University, Sweden*, “Quantum Kinetic Models in Plasmas Including the Effects of the Electron Spin” 8

11:50 Ian Welland and D. K. Ferry, *Arizona State University, USA*, “Wigner Function in Quantum Photonic Processing” 10

12:10 *Lunch*

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- 2:45 *General discussion and questions*
- 3:00 Josef Weinbub¹, Mauro Ballicchia², David K. Ferry³, and Mihail Nedjalkov¹, ¹*Institute of Microelectronics, TU Wien, Austria*, ²*Universita Politecnica delle Marche, Italy*, ³*Arizona State University, USA*, “Electron Interference and Wigner Function Negativity in Dopant Potential Structures” 14
- 3:20 Maciej Woloszyn and Bartłomiej J. Spisak, *AGH University of Science and Technology, Poland*, “The Wigner Monte Carlo Approach to Transport Characteristics of Nanodevices” 16
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- 4:00 Maarten L. Van de Put¹, Bart Sorée^{2,3,4}, and Wim Magnus³, ¹*University of Texas at Dallas, USA*, ²*IMEC, Belgium*, ³*University of Antwerp, Belgium*, ⁴*KU Leuven, Belgium*, “Wigner Time-Evolution Using the Spectral Components of the Force” (Invited) 18
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³*Bulgarian Academy of Sciences, Bulgaria*, ⁴*Arizona State University,
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Quantum Mechanics of Anything (From Qubits to Atoms and Molecules) as a Statistical Theory (i.e. in Phase Space)

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We present a complete phase-space formulation of quantum mechanics - extending work by Wigner, Weyl, Moyal, and others to any quantum system. This talk is structured in three parts. I will start by presenting a brief introduction and outline of the formalism. This will be followed by a number of example applications visualising the quantum properties of qubit, atom-field and atomic systems. I will conclude with a summary of some key historical developments in the subject and specific mathematical details of the general formalism.

Microcanonical Centroid Framework and the Wigner Distribution

Lindsay Orr¹, Lisandro Hernández de la Peña², and Pierre-Nicholas Roy¹

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The path integral representation of quantum statistical mechanics introduced by R. P. Feynman renders an ideal setting for the description of many-particle systems in canonical equilibrium.[1] While static properties are immediately available in this context, dynamical properties (via quantum time correlation functions) can be estimated within the linear response theory regime using the notion of a path centroid variable, as shown by Jang and Voth.[2] In this work, we extend the Feynman centroid approach to the analysis of systems in microcanonical equilibrium.[3] We define a general mapping of quantum mechanical operators onto centroid phase space and establish how to recover quantum mechanical information through classical-like, phase-space averages. We show how to extract equilibrium properties and demonstrate that the underlying quantum dynamics is rigorously connected, within this formalism, to double Kubo transform quantum time correlation functions. The central quantity within this framework, the centroid density, is shown to be closely related to the corresponding Wigner function of the ensemble and turns precisely into the Wigner function at a particular limit. A Centroid Molecular Dynamics (CMD) approximation to the exact quantum dynamics is proposed and proven exact in the harmonic limit. This approach is tested numerically, and compared with exact results, for a quartic oscillator and a double-well potential. In the case of ground state dynamics, we show that this method can resolve tunneling splittings of the double well problem in the higher barrier regime where other approaches are likely to fail.

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S. Jang and G. A. Voth, *J. Chem. Phys.*, **111**, 2371 (1999)

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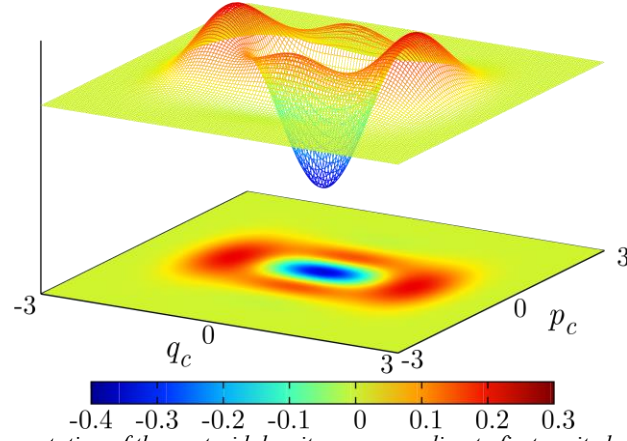


Fig. 1: Phase-space representation of the centroid density corresponding to first excited state of the double well potential at $\beta = 1$.

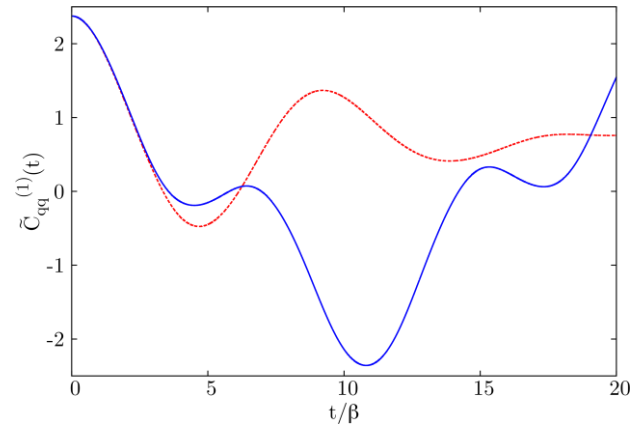


Fig. 2: Exact (blue) and CMD results (red) for the position-position double Kubo quantum time correlation function corresponding to the first excited state of the double well potential at $\beta = 1$.

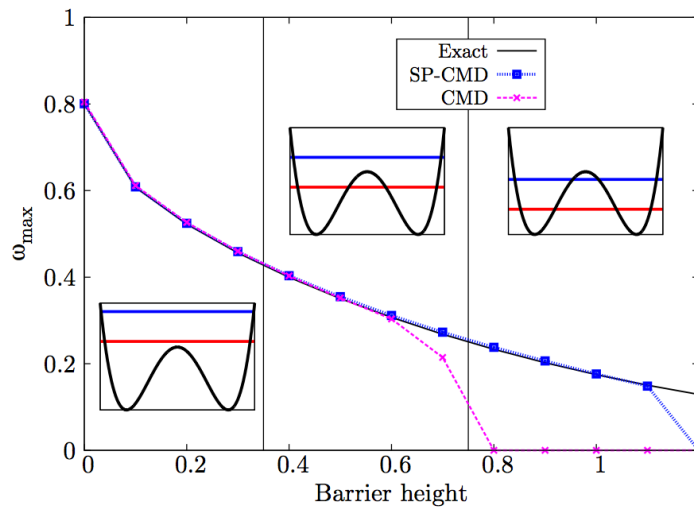


Fig. 3: Energy gap between ground state and first excited state of a double well potential as a function of the barrier height. The results shown are: exact (black solid line), microcanonical CMD (blue dotted line with squares) and canonical CMD (purple dashed line with crosses). The inserts denote schematically the three different tunneling regimes exhibited by this system.

Dynamics of the Wigner Distribution Function on the Bunimovich Stadium

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Currently, electronic nanosystems are objects of intensive experimental and theoretical research in basic science and engineering. The interest in these systems results from the fact that they are examples of artificial systems in which quantum phenomena are enhanced by the quantum size effect. Computer simulations are an indispensable element of this kind of research because optical and transport properties of these nanosystems can be inferred before the experimental verifications.

In this short report we present preliminary results of our studies concerning the quantum dynamics of the electronic state in the planar bounded domain which consists of a rectangle bounded at both ends by semicircles. In the classical mechanics such system is called the Bunimovich stadium [1, 2] and belongs to the class of simple systems which display a chaotic dynamics. Our studies of the properties of the system are based on the phase-space formulation of quantum theory [3]. In this framework the system is characterized by the Weyl symbol of the Hamiltonian, and the states are represented by c -number functions of the position and momentum variables which are called the quasi-distribution functions. One of them is the Wigner distribution function (WDF) which is defined by the inverse Weyl transform of the density operator [4]. Equation of motion for the WDF can be written in the form of the (2+2)-dimensional integro-differential equation with the non-local integral kernel. The equation augmented by the initial condition in the form of the Gaussian wavepacket is solved using the ViennaWD package with the reflecting boundary condition. The operation of this package is based on the stochastic Wigner Monte Carlo method using the signed-particle technique [5, 6]. As a result of our studies of the Bunimovich stadium we present some dynamical characteristics of the system and discuss them in the context of non-classicality.

Acknowledgments. This work was partially supported by the Faculty of Physics and Applied Computer Science AGH UST statutory tasks within subsidy of Ministry of Science and Higher Education.

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Non-Linear Wave Damping due to Multi-Plasmon Resonances

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Classically, waves in plasmas can be damped through interaction with particles with velocities close to the phase velocity, if there are any [1]. A quantum treatment using the Wigner-Moyal equation instead predicts, in linear theory, a resonance offset from the phase velocity by $v_q = \hbar k / 2m$ where \hbar is the reduced Planck constant, k is the wavenumber and m is the electron mass [2]. We demonstrate that in non-linear theory, there are resonances offset by nv_q for any integer n [3]. The non-linear ($n \geq 2$) resonances can be interpreted as absorption/emission of multiple plasmon quanta, and we term them *multi-plasmon resonances*. If the linear resonance ($n = 1$) is in the tail of the electron distribution, the multi-plasmon processes may be comparable or stronger, due to a much larger number of electrons participating. This is especially the case for highly degenerate electrons if the $n = 1$ resonance is just outside the Fermi sphere, see Fig. 1. We derive evolution equations for the electron distribution and wave amplitude. The key step is dividing the phase space into resonant and non-resonant regions [4], where non-linear effects are important only in the former. Solving our equations numerically, we find the expected wave damping, with damping rate comparable to that from linear theory [5].

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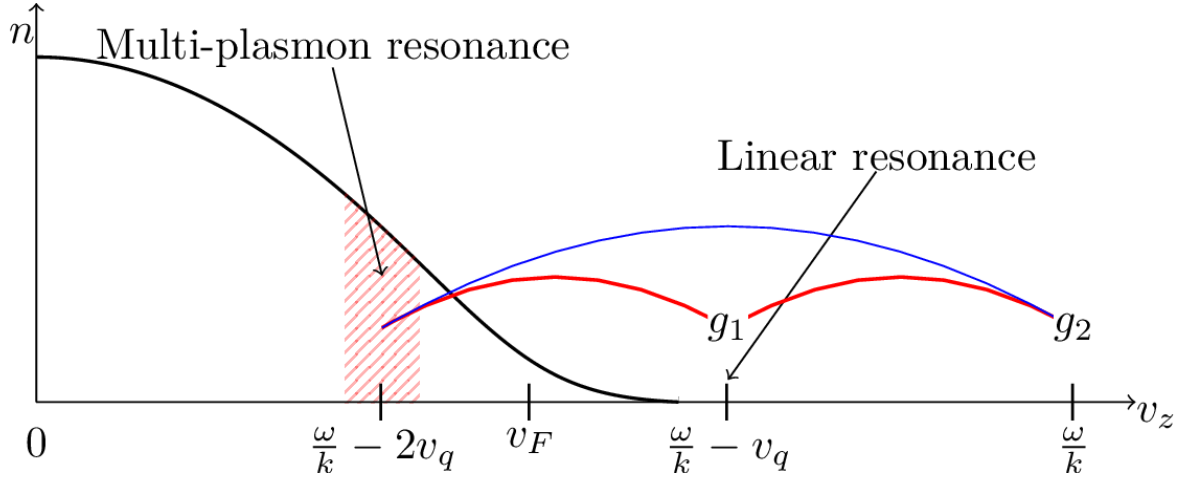


Fig. 1: The two-plasmon resonance in a Fermi-Dirac distribution at $T = 0.2 T_F$. The red (blue) lines represent absorption/emission of plasmon quanta at the fundamental frequency (second harmonic). Since there are many more particles near the multi-plasmon resonance than near the linear resonance, the two-plasmon process can be at least as important as the single-plasmon process.

Quantum Kinetic Models in Plasmas Including the Effects of the Electron Spin

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Many plasmas in laboratory and space can be treated classically. However, when the nearest neighbor distance between electrons become of the order of the thermal de Broglie wavelength or smaller, quantum effects become important, see fig. 1 for details. A quantum kinetic description of electrons can then be devised with the help of the Wigner transform but the standard treatment only covers the most basic quantum properties, as described by the Schrödinger equation. When the dynamics related to the electron spin becomes significant, a more elaborate treatment is needed, based on the Pauli equation or – if relativistic effects should be covered – the Dirac equation. Recently a quantum kinetic model for electrons was derived based on the Pauli equation by combining the ordinary Wigner transformation by the so-called Q-transformation [1]. The model uses the spin state as an extra independent variable and covers quantum properties such as particle dispersive effects, spin magnetization, the magnetic dipole force, and spin precession. While this model predicts several new phenomena, e.g. resonances and wave modes that do not appear in classical theory, it does not include relativistic physics. An extended approach, based on the Dirac equation, was conducted in Ref. [2], which covered also electric polarization due to the spin and spin-orbit interaction. The derivation still involved weakly relativistic approximations and a further generalization to allow for a fully relativistic theory was performed in Ref. [3]. Interesting results due to the relativistic approach is, for example, the non-trivial relation between momentum and velocity that depends crucially on the spin state. A drawback present in Refs. [2,3] but not in [1], is the limitation to scale lengths much longer than the characteristic de Broglie length. A model combining the virtues of Refs. [1] and [2] allowing for both weakly relativistic effects and short scale lengths is under development.

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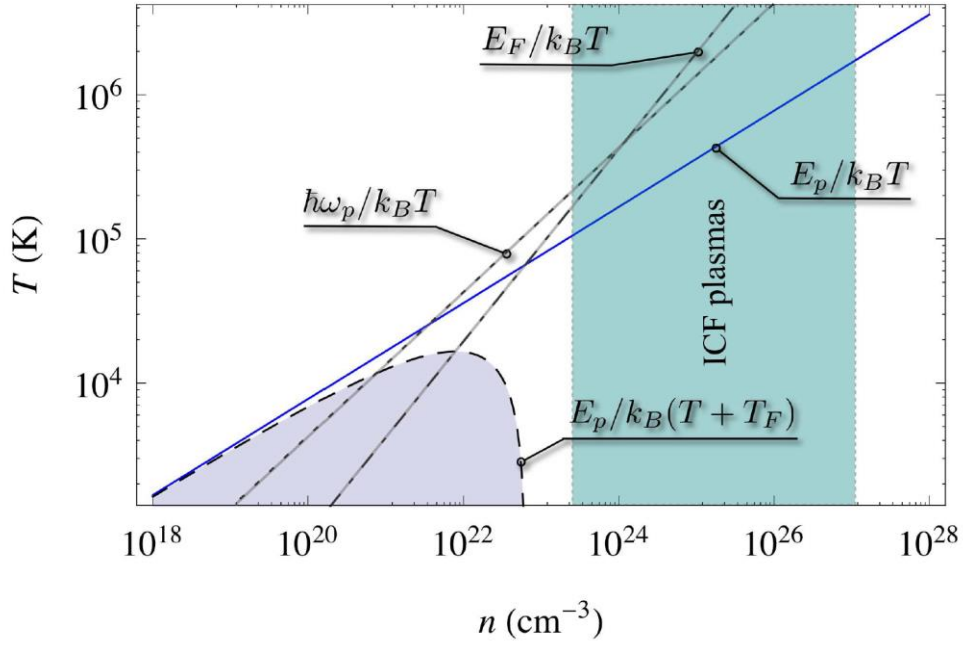


Fig. 1:

Different plasma regimes in the temperature-density parameter space. The dotted line is where the strong coupling parameter $\Gamma = E_p/k_B T = 1$, where E_p is the potential energy due to the nearest neighbor. For higher densities the average kinetic energy of the particles is given by the Fermi energy $k_B T_F$ rather than the thermal energy and the strong coupling parameter must be replaced by $\Gamma_F = E_p/k_B(T + T_F)$. In this graph $\Gamma_F = 1$ is illustrated by the dashed curve, and the strong coupling region (shaded) lies below this line. Here higher order correlations (collisions) have to be taken into account, and the mean-field description is not valid. For comparison, the lines $\hbar\omega_p/k_B T = 1$ (dotted gray line), where $\hbar\omega_p$ is the plasmon energy and T_F/T (dotted-dashed gray line) are also plotted. These measure, respectively, the relative importance of wave function dispersion and the Fermi pressure. As a rough estimate, the quantum regime lies below these lines. The area marked ICF denotes the regime of relevance for inertial confinement fusion experiments.

Wigner Functions in Quantum Photonic Processing

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Quantum entanglement is at the heart of information and computing technology proposed for the coming generations. One approach lies in the use of quantum optics for the production of qubits in these applications [1,2]. The presence of nonlinearities in Si waveguides [3,4] and ring resonators [5,6] can lead to entangled photon generation by four-wave mixing. In this process, two source photons are absorbed and two new photons at the signal and idler frequencies are created. The Wigner function is extremely useful in illuminating the physical processes and the entanglement arising from the optical interactions. Here, we begin to study the nonlinear optical processes by considering the coupling between a dielectric wave guide and a ring resonator, considering pulse optical sources at 1.5 μm and a Si waveguide of width and height $0.5 \times 0.22 \mu\text{m}$. The excitation is considered in terms of the transverse wave function defined by the TE_1 mode at the laser frequency, and a longitudinal Wigner function whose spatial and momentum spread are also determined from the pulse parameters. We study propagation of the Wigner function including the waveguide dispersion, coupling between the waveguide and the ring resonator and interaction between various optical waves.

Acknowledgments. Funding from the Arizona Regents' Initiative Fund, project 460929, is acknowledged.

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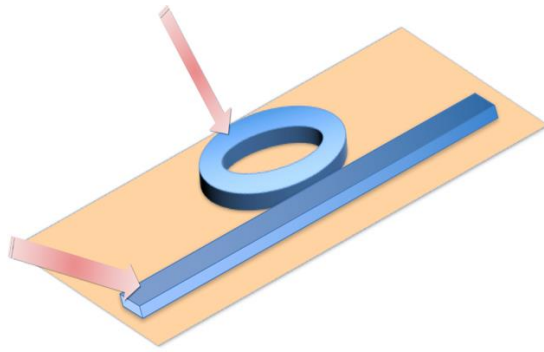


Fig. 1: The Si waveguide and ring resonator are shown with sites of laser illumination..

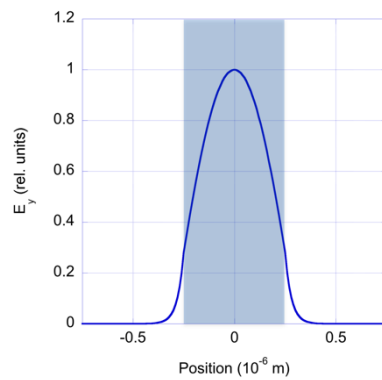


Fig. 2: Transverse E_y profile for the TE_1 mode at $1.5 \mu\text{m}$. The width of the waveguide is overlaid on the figure by the shaded area. The position is the lateral x-dimension.

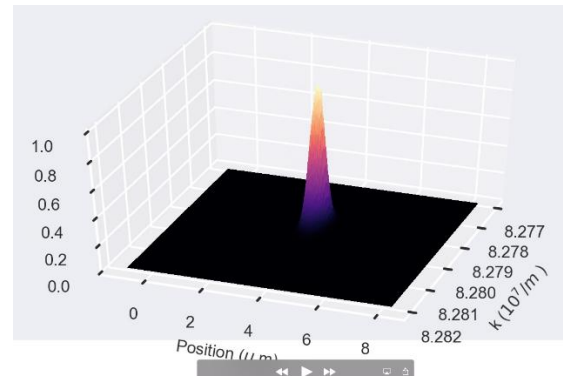


Fig. 3: Gaussian for a 6 ps optical pulse at $1.55 \mu\text{m}$ in the silicon waveguide. The initial pulse, and Wigner function, are classical at this point.

Squeezing and Entanglement in Electron Quantum Transport

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A classical current in a conductor radiates a classical electromagnetic field. We explore some properties of the field radiated by a conductor when electron transport must be described by quantum mechanics, i.e. when the electron current becomes quantum itself. Using a tunnel junction between normal metal contacts placed at ultra-low temperature as a quantum conductor, we demonstrate the existence of squeezing as well as entanglement in the microwave radiation, thus proving that the electron shot noise generates a quantum electromagnetic field [1,2]. This is corroborated by the direct demonstration of photon pairs emitted by the sample [3,4].

Beyond these experiments, which have been performed in frequency domain by measuring quadratures of the electromagnetic field at two frequencies (see corresponding Wigner functions in Fig. 1), it is tempting to address quantum properties of the electromagnetic field not at a given frequency but at a given time. Indeed, electron transport in quantum conductors often bears no intrinsic timescale, thus no preferred frequency. As a consequence, quantum correlations in the radiated field are extremely broadband. This comes from the statistics of current fluctuations, whose correlations can be clearly understood in time domain.

We will discuss very recent theoretical results which aim at understanding quantum electromagnetic fields in time domain, such as quadratures or photon statistics [5].

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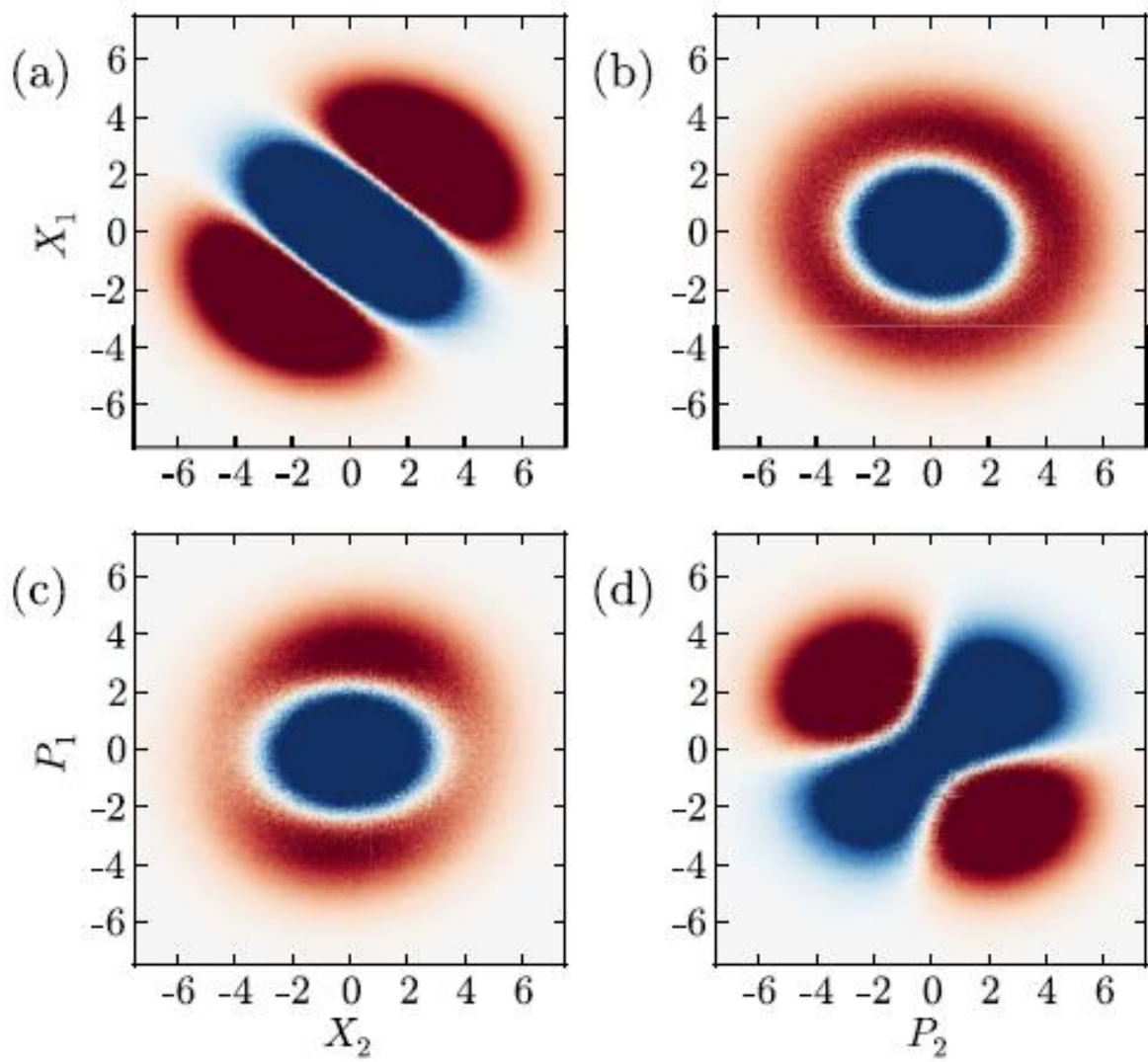


Fig.1: Probability distribution of the quadratures of the current fluctuations measured at frequencies $f_1=7$ GHz and $f_2=7.5$ GHz. The sample is a tunnel junction placed at ultra-low temperature $T=15$ mK, biased by a DC voltage and an ac excitation at 14.5 GHz.

Electron Interference and Wigner Function Negativity in Dopant Potential Structures

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²*Institute for Microelectronics, TU Wien, Austria*

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We present two experiments in quantum current transport concerning interference effects and the use of Wigner function negativity: (1) We show interference effects as a result of the electron evolution within a coherent transport medium, offering a double-dopant Coulomb potential structure [1]. (2) We discuss the relation between quantum coherence and quantum interference and the negative parts of the Wigner quasi-distribution in a single-dopant Coulomb potential structure [2]. Injections of coherent electron states into the structures are used to investigate the effects on the current transport behavior within the quantum Wigner phase space picture [3,4]. Quantum effects are outlined by using classical simulations as a reference frame, a unique feature of Wigner function based transport simulations. In particular, the signed-particle approach inherently provides a seamless transition between the classical and quantum domain. Based on this we are able to identify the occurring quantum effects caused by the non-locality of the quantum potential, leading to spatial resonance. Fig. 1 and Fig. 2 show the electron density at 200 fs for all absorbing boundary conditions (i.e. an open system) in the classical and in the quantum case, respectively. In the classical case, Fig. 1, no interference pattern materializes beyond the dopants as the action of the force is local. In the quantum case, Fig. 2, the non-locality action of the quantum potential of the dopants affects the injected electrons already right after injection and establishes two *transport channels* below the dopants. Beyond the dopants (i.e. $y > 30$ nm), interference effects manifest which are highly sensitive to changes of the dopants' potential profiles. The results bear a resemblance to the diffraction patterns manifesting over time in double-slit experiments [5,6] and depict the use of dopants to design transport channels as well as specific interference patterns within an open system. In another experiment, a single repulsive dopant is placed in the transport path of an *open* structure (using absorbing lateral boundary conditions) which creates a quasi-two-slit electron system that separates the wave function into two entangled branches. Here, the negative part of the Wigner function is principally concentrated in the region behind the dopant between the two entangled branches, maintaining the coherence between them (Fig. 3). Moreover, quantum interference is shown in this region both in the negative and in the positive part (Fig. 4). Both experiments are essential steps towards novel applications in the area of entangletronics [1,7].

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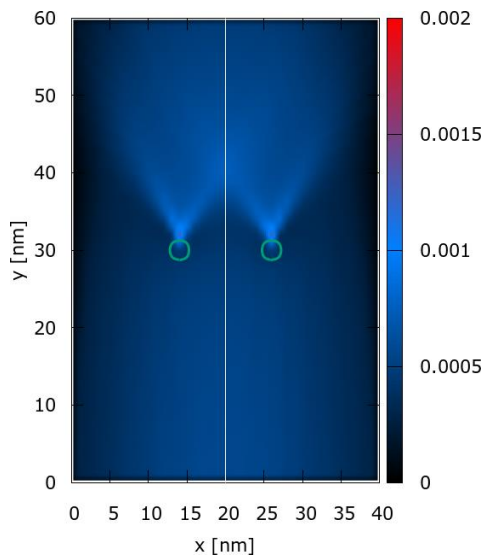


Fig. 1: Classical electron density ([a.u.]) after 200 fs of the initial minimum uncertainty condition using absorbing boundary conditions (green circles: Coulomb potentials).

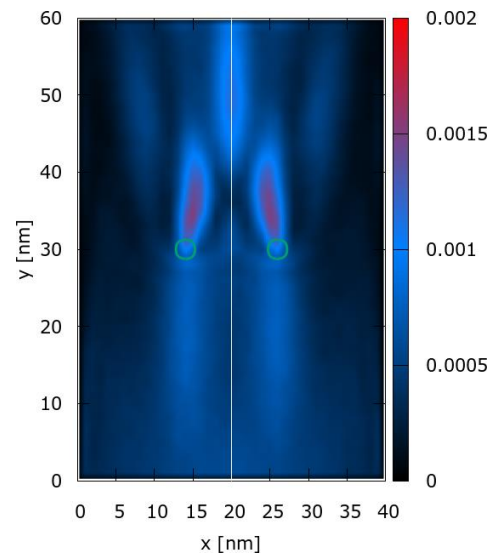


Fig. 2: Quantum electron density ([a.u.]) after 200 fs of the initial minimum uncertainty condition using absorbing boundary conditions (green circles: Coulomb potentials).

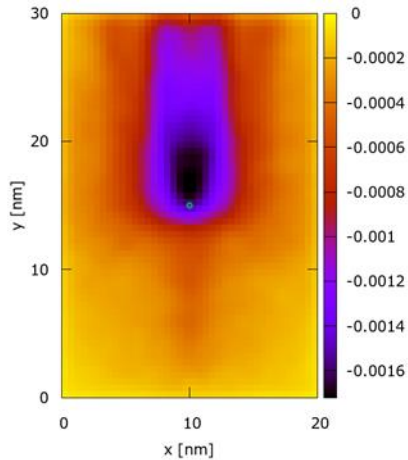


Fig. 3: Spatial distribution of the negative part of the Wigner distribution.

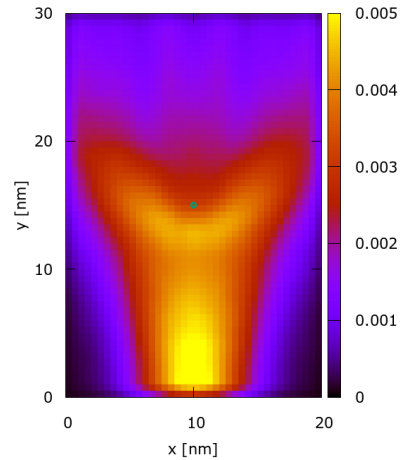


Fig. 4: Spatial distribution of the positive part of the Wigner distribution.

The Wigner Monte Carlo Approach to Transport Characteristics of Nanodevices

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The quantum kinetic methods based on the Wigner distribution function and its equation of motion are one of the powerful methods of investigating the transport properties of electronic systems or nanosystems[1]. This particular approach allows us to have a unique insight into the dynamics of such processes and into the details of quantum phenomena taking place during the system evolution. However, those possibilities do not come without cost. The price that must be paid is the numerical complexity of finding the solution in virtually all non-trivial cases. Direct approaches based on the discretization of the Wigner Transport Equation[2] are therefore in practice limited to one-dimensional problems. Yet the realistic simulations of nanodevices require two- and three-dimensional formulation, which leads to four- or six-dimensional problems in the phase space, plus the time dependence.

Those limitations may be overcome with help of the Monte Carlo methods based on the signed particle approach[3,4], which not only allows using the Wigner approach in more than one dimension, but also makes it possible to include factors like e.g. scattering or surface roughness[5]. In this report we analyze the possibilities of Monte Carlo calculations which result in finding transport characteristics such as the current-voltage dependencies, in the case of typical systems like e.g. the double-barrier devices used as resonant tunneling diodes[6-9], using the ViennaWD software[10].

Acknowledgments. This work was partially supported by the Faculty of Physics and Applied Computer Science AGH UST statutory tasks within subsidy of Ministry of Science and Higher Education.

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Wigner Time-Evolution using the Spectral Components of the Force

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In this talk, we present an alternative formulation of the Wigner-Liouville equation that is based on the spectral components of the classical force instead of the potential energy as detailed in Ref. [1]. The standard Wigner-Liouville equation, describing the coherent time-evolution of the Wigner function, is known to be a highly oscillatory integro-differential equation that acts non-locally in both space and momentum. Our formulation, on the other hand, can be interpreted intuitively as a density-conserving, local generation process and readily admits a direct numerical implementation.

To recast the Wigner-Liouville equation, we decompose the classical force field into its Fourier components, $F(x) = \sum_k \tilde{F}_k e^{ikx} = \sum_k F_k(x)$. This decomposition allows for the recasting of the Wigner-Liouville equation in 1D as a particularly simple equation that bears resemblance to the classical Boltzmann transport equation (Vlasov equation):

$$\frac{\partial}{\partial t} f(x, p, t) + \frac{p}{m} \partial_x f(x, p, t) + \int dk \frac{F_k(x)}{\hbar k} \left[f\left(x, p + \frac{\hbar k}{2}, t\right) - f\left(x, p - \frac{\hbar k}{2}, t\right) \right] = 0$$

We find that the last term, that captures the quantum mechanics, acts as a local, density conserving, generation rate of positive and negative ‘probability’ to states with momentum $\pm \hbar k/2$, as illustrated in Fig. 1. This interpretation is similar to the generation of signed particles in the Monte-Carlo implementation of the Wigner equation [3]. However, our reformulation, and its interpretation as a generation process, facilitates a direct numerical implementation. In particular because the factor $1/k$ provides a natural damping of the high wavevector components of the force field. We demonstrate the method using two implementations based on pseudo-spectral methods, as well as a semi-Lagrangian scheme. Both methods minimize numerical diffusion, a necessity to simulate coherent quantum transport over significant time periods.

In Fig. 2, we show coherent reflection of a wavepacket on a single barrier, demonstrating the stability and accuracy of our method. In Fig. 3, we show transfer characteristics of a resonant tunneling diode (RTD) obtained using Wigner time-evolution [1]. In Fig. 4, we compare the Wigner method to a wavefunction based method for a fixed-potential RTD structure [4].

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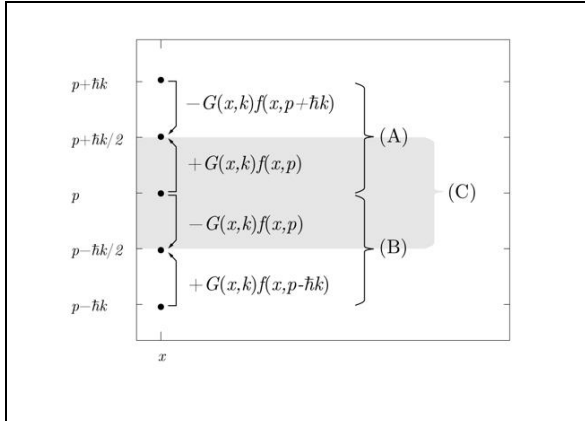


Fig. 1: Particle conserving generation process (C) of positive and negative quasi-probability from momentum p to $p \pm \frac{\hbar k}{2}$ with a generation rate given by $G(x, k) = \frac{F_k(x)}{\hbar k}$. Process (C) emerges from processes (A) and (B), as in the equation given on the previous page.

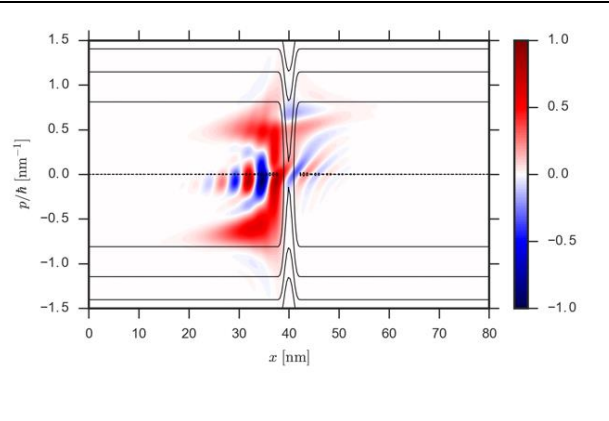


Fig. 2: The Wigner function of a wavepacket with average wavevector 0.5 nm^{-1} upon collision with a single barrier at 40 nm. The classical trajectories (iso-energy lines) are shown as black lines.

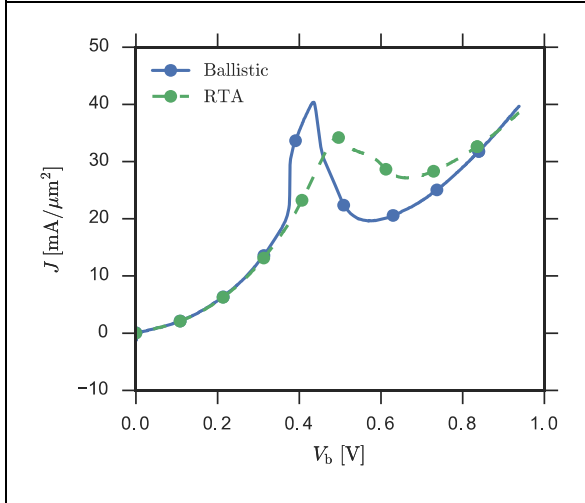


Fig. 3: The transfer characteristics for a resonant tunneling diode obtained using the self-consistent Wigner time-evolution. Lines: continuous plot of the current while doing an adiabatic sweep of the bias. Points: Time-evolution to steady state. Fully coherent (Ballistic) and with the relaxation time approximation (RTA).

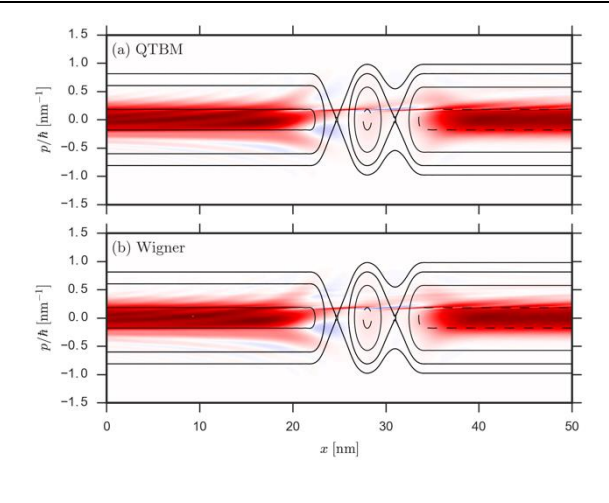


Fig. 4: The Wigner function of (a) a ballistic wavefunction based calculation using the quantum transmitting boundary method (QTBM) and (b) the steady state of a coherent Wigner time-evolution simulation, starting from a uniform Fermi-Dirac distributions. The classical trajectories (iso-energy lines), indicating the position of the barriers, are shown as black lines.

Wigner-Boltzmann Transport Simulation for Improving the Thermoelectric Power Factor in 2D Materials

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Thermoelectric (TE) energy conversion has attracted interest as a way to improve the efficiency of power generation by converting waste heat in to electricity. Higher power factor combined with lower thermal conductivity help to improve the TE conversion efficiency; achieving both simultaneously is challenging and typically requires nanostructured and highly doped semiconductor materials. Several studies showed that energy filtering of carriers, implemented in the form of single and multiple potential barriers in nanocomposites, heterostructures, and superlattices, is an effective way to improve power factor [1, 2]. The challenge in modeling nanostructured TE materials and devices is in capturing both quantum effects, such as tunneling through energy barriers, and “semi-classical” effects like electron-phonon and impurity scattering. In our previous work [3], we developed an iterative solver for the Wigner-Boltzmann transport equation. We studied the impact of the spatially varying potential barriers in silicon, both superlattices and nanowires, and concluded that sharp, tall barriers with small periods result in higher power factors and therefore better TE performance.

In this work, we extend our 3D model to simulate quantum transport and capture energy filtering in 2D material in order to evaluate their potential for TE applications. We focus on single-layer (SL) molybdenum disulfide (MoS_2) [4] as it possesses a bandgap, and introduce potential barriers (Figure 1). The band structure of MoS_2 is calculated from first principles while transport is captured in the Wigner-Rode formalism. TE parameters are calculated for SL MoS_2 and found to reproduce the intrinsic behavior (Fig. 2). Then the potential barriers are introduced in SL MoS_2 to study their influence. Energy relaxation and quantum effects from periodic spatially varying potential barriers are modeled using the Wigner-Rode formalism [3]. At higher period lengths (L_p), an increase in the amplitude of the applied potential V_0 , Seebeck coefficient (S) increases and electrical conductivity (σ) decreases due to thermionic emission of carriers. Reducing L_p results in reduction of S for square barriers. An effect of additional quantum reflections that arise in the square barriers that leads to higher tunneling (Fig. 4). Power factor increases in square barriers with lower period lengths that are asymmetric (Lower or higher duty cycle, α), and little or no effect on power factor at high period lengths (Fig. 5). Our comprehensive Wigner-Rode transport model showed an increase in power factor for both cosine and square barriers in SL MoS_2 with the height of the potential barrier and at least 30% enhancement (Fig. 6). Further investigation into understanding the effect of multi-barrier structures will create efficient TE devices for future applications.

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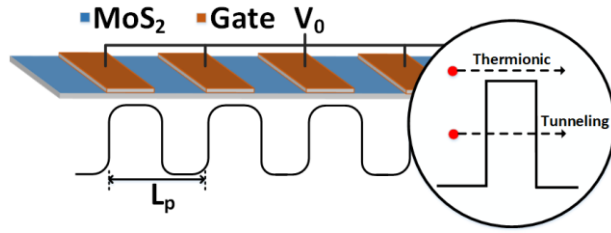


Fig. 1: Schematic of the simulated structure to study energy filtering in SL MoS₂ with a series of spatially varying potential barriers.

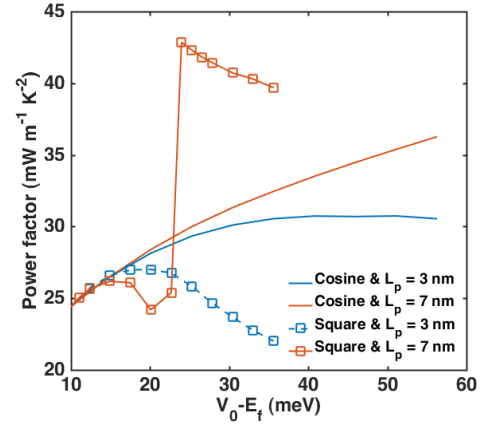


Fig. 4: Effect of barrier periodic length (L_p) on TE parameters showing the impact of tunneling in low period lengths.

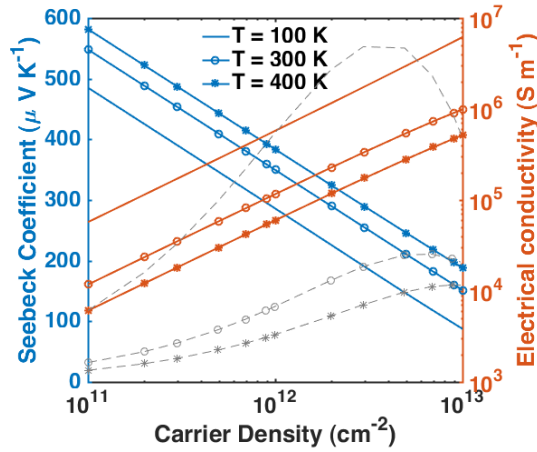


Fig. 2: S and σ for SL MoS₂ at different temperatures by varying the carrier density. Power factor is plotted (light gray) to identify the maximum with respect to applied carrier density.

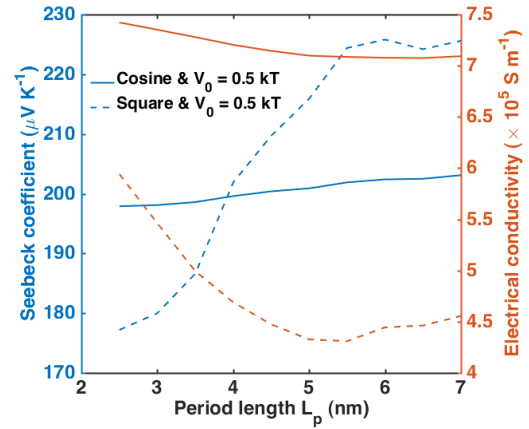


Fig. 5: Effect of square potential barrier duty cycle (α) on power factor at both $L_p = 3$ nm and $L_p = 7$ nm. Here the barrier height of 0.4 kT corresponds to $V_0 - E_f$ of 20 meV and 1 kT to 35 meV. The simulations are performed at a carrier density of $7 \times 10^{12} \text{ cm}^{-2}$ and a temperature (T) of 300 K.

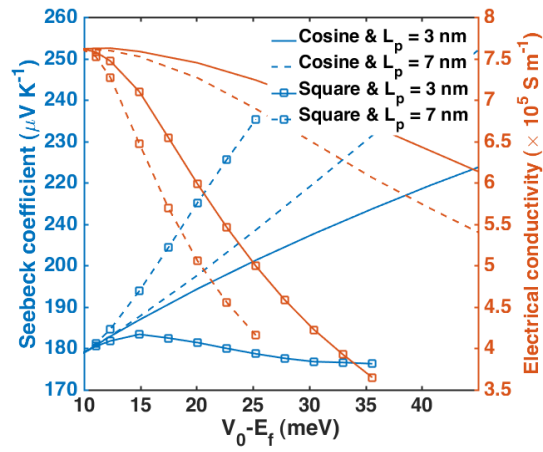


Fig. 3: Effect of potential barrier amplitude (V_0) on S and σ . The simulations are performed at a carrier density of $7 \times 10^{12} \text{ cm}^{-2}$ and a temperature (T) of 300 K.

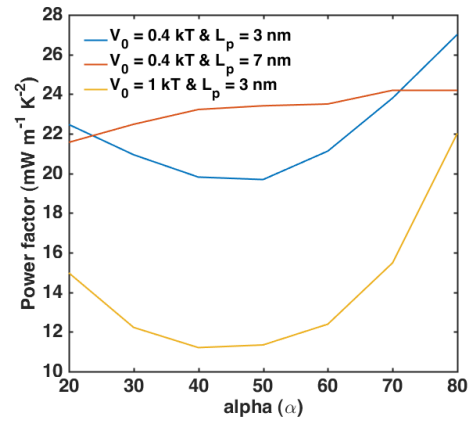


Fig. 6: Power factor enhancement in SL MoS₂ due to the energy filtering from potential barriers.

Wigner Function Negativity as a Resource for Quantum Computation

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This talk is concerned with Wigner functions in finite-dimensional state spaces and their role in a particular scheme of universal quantum computation, so called quantum computation with magic states. Such computational schemes can be classified by the Hilbert space dimension d of the local constituent systems (qudits). As it turns out, there is a difference between odd and even d . Namely, if d is odd, then the finite-dimensional case looks very similar to the original infinite-dimensional case; but if d is even then there are severe difficulties to overcome. Those difficulties originate from Mermin's square and star, two simple proofs of contextuality of quantum mechanics.

My talk will have a review part and a research part. In the former, I'll describe (a) D. Gross' adaption of the original Wigner function to odd finite dimension [1], (b) Clifford gates and the Gottesman-Knill theorem, (c) Quantum computation with magic states [2] and the role of Wigner function negativity therein [3], and (d) the relation between Wigner function negativity and contextuality of quantum computation [4].

In the research part, I discuss work on the case of even d , specifically $d=2$. There is a construction for rebits which gets around the difficulties posed by Mermin's square and star [5]. Time permitting, I will also discuss the full qubit case in which there is no way around Mermin's square and star. We introduce a novel quasiprobability distribution which reduces to Gross' Wigner function for odd d , but looks quite different for $d=2$. It is covariant under all Clifford gates and positivity-preserving under all Pauli measurements. In result, we establish negativity of this quasi probability distribution as a necessary prerequisite for a quantum speedup, completely analogous to the case of odd d .

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Electron Evolution and Boundary Conditions in the Wigner Signed-Particle Approach

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In modern nanoelectronics understanding quantum current transport is a fundamental challenge. In turn, in quantum mechanics evolution is driven by all the derivatives of the electric potential so rapid spatial variations of the potential can determine non-local effects, tunneling, and also interference phenomena. Those effects give rise to a complex interplay and cannot be decomposed in elementary processes to analyze separately. Thus, numerical modeling is a fundamental tool for studying quantum phenomena, since it allows to consider specific conditions that are difficult to implement by experimental approaches, e.g., switching between different boundary conditions to see how this affects the electron evolution [1] or de-activating scattering events [2]. The Wigner formulation of quantum mechanics provides a seamless transition to classical evolution, that represents a reference to highlight quantum effects [3]. In the signed-particle approach [4], electron evolution is modeled by the evolution of numerical particles that move along Newtonian trajectories and carry a sign. This aspect simplifies the implementation of “classical” boundary conditions, generally unfeasible in practice experimental approaches. We analyze the electron evolution against a repulsive dopant with a maximum potential energy of 0.175 eV with two different lateral boundary conditions [5]: absorbing boundaries, Fig. 1, and perfect reflecting boundaries, Fig. 2. From the comparison between the quantum electron density, Fig. 1b), and corresponding classical counterpart, Fig. 1a), we can notice the non-locality effects before and around the dopant, and also the tunneling that increased the quantum electron density in front of the dopant. Fig. 3a) shows the ratio between quantum and classical electron density, allowing to witness both the decrease below unity due to nonlocal effects and the peak in front of the dopant that reaches the maximum of 14 due to tunneling effects. In Fig. 2a) and Fig. 2b), we show the same scenario but for lateral reflecting boundaries. The electrons reflected from the lateral boundaries, both in the quantum and in the classic case, are injected in front of the dopant but in the quantum case the electron density is much more closed around the dopant due to the interplay of the non-locality and tunneling effects. As shown in Fig. 3b), the quantum density continues to be greater than the classic one in front of the dopant but now limited to a factor of 3 since the electrons reflected by the boundaries mitigate the effect of tunneling.

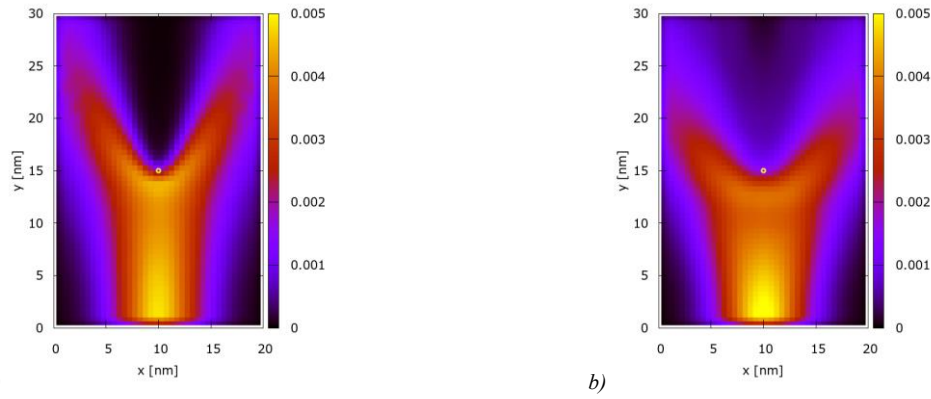


Fig. 1: Electron density around the dopant with 0.175 eV peak energy (yellow isoline represents the 0.15 eV level) with lateral absorbing boundary condition: a) classical evolution, b) quantum evolution.

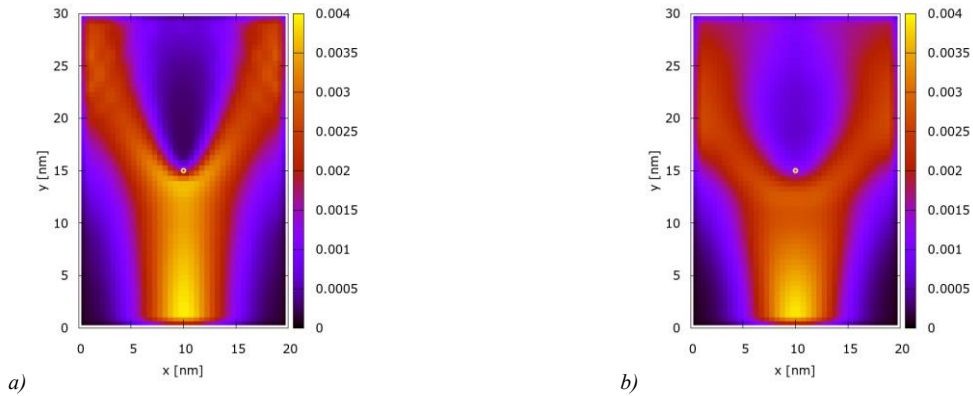


Fig. 2: Electron density around a dopant with 0.175 eV peak energy (yellow isoline represents the 0.15 eV level) with lateral reflecting boundaries: a) classical evolution b) quantum evolution.

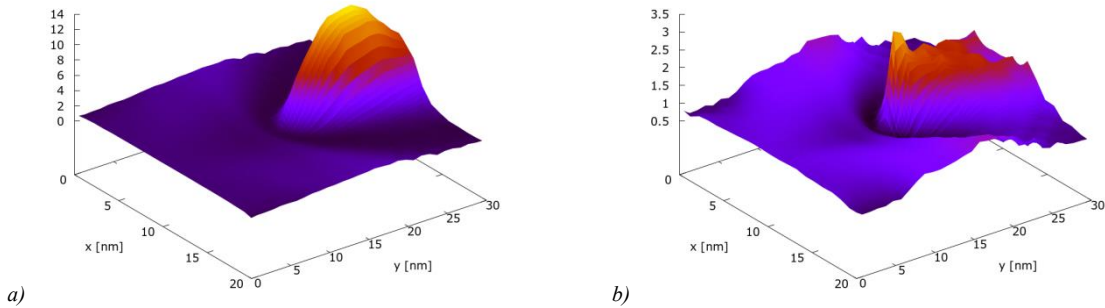


Fig. 3: Ratio between quantum and classical electron density: a) lateral absorbing boundaries, b) lateral reflecting boundaries.

Acknowledgments: The financial support by the Austrian Science Fund (FWF) project FWF-P29406-N30, the Austrian Federal Ministry of Science, Research and Economy, and the National Foundation for Research, Technology and Development is gratefully acknowledged. The computational results presented have been achieved using the Vienna Scientific Cluster (VSC).

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On the Incompatibility Between Frensley's Inflow Boundary Conditions and Stationary Wigner Distribution Functions: The Problem and the Solution

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The simulation of electron devices requires a partition between an active region (open system) and the reservoirs. The Wigner distribution function, dealing with the phase-space of open quantum systems, has a large tradition in the simulation of quantum electron devices, but it requires reasonable physical arguments to fix the properties of electrons at the spatial borders of the active region. To guarantee irreversibility, Frensley suggested the reasonable assumption of treating the reservoir as a blackbody; he assumes that the distribution of electron emitted into the device is described by the thermal equilibrium distribution function of the reservoir, while the outflowing electrons are absorbed without reflection [1]. This translates into fixing entirely the Wigner distribution function for all positive (negative) momenta at the left (right) border of the active region.

The problem discussed in this conference appears because the definition of the momentum of the Wigner distribution function - through a Wigner-Weyl transformation - is not the same as the orthodox one. Although its marginal probability coincides, the former momentum depends on position, while the latter does not. We show that this mathematical incompatibility can have dramatic consequences in time-independent scenarios, as for scattering states in a single/double potential barrier (Fig.1). An electron injected from the left with a well-defined positive orthodox momentum (green triangle in Fig.2) induces additional unexpected inflowing Wigner-Weyl momenta at the left boundary. The situation is even more dramatic when dealing with a resonant state, where an electron with positive orthodox momentum at the left, induces unexpected inflowing negative Wigner-Weyl momenta at the right (Fig.3). In the literature, the solutions to this incompatibility is either criticizing the Frensley's boundary conditions [2] or looking for a new phase-space distribution [3].

On the contrary, we show that this apparent incompatibility is simply solved by using time-dependent approaches [4]. Here, electrons are defined as wave-packets with a spatially limited quantum non-locality (Fig. 4), while scattering states have infinite non-locality. We show that this localization prevents spurious Wigner-Weyl momenta to arise at the interfaces (Fig. 5-6), and lead to a successful compatibility between the natural Frensky's boundary conditions and time-dependent Wigner distribution functions (with or without irreversible phenomena).

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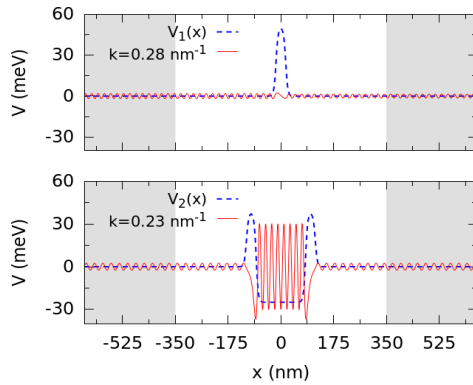


Fig. 1: Stationary states (red solid line) of a single-electron with well-defined injected momentum for a single (top) and double (bottom) potential barrier (blue dashed line).

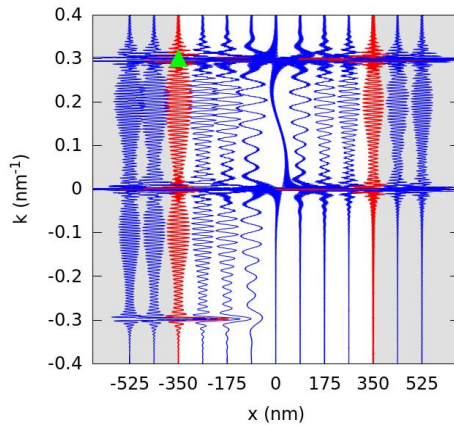


Fig. 2: Wigner distribution function at fixed coordinates for the single state of Fig. 1 (top). The grey areas define the interface with electronic reservoir, where the single-electron mode (green triangle) is injected.

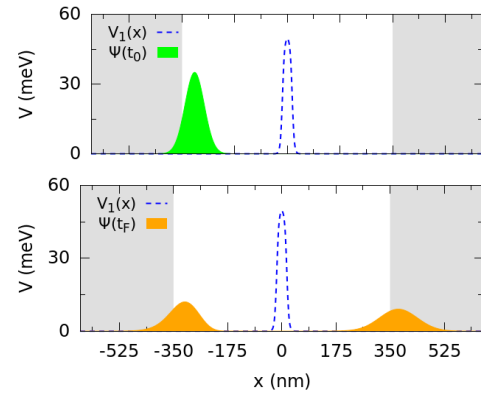


Fig. 4: Dynamical wave function at initial (top) and final (bottom) time of the single-electron in presence of a single potential barrier (blue dashed line).

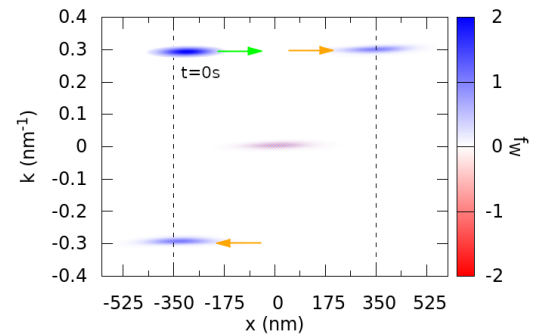


Fig. 5: Time dependent Wigner distribution function at the final time for the wave packet evolution of Fig. 4. The label $t=0$ shows the natural Wigner distribution function at the initial time.

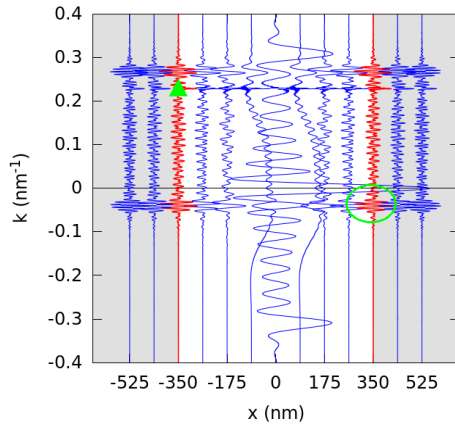


Fig. 3: Wigner distribution function at different fixed coordinates for the resonant state of Fig. 1 (bottom). Negative Wigner-Weyl momenta are present at the right interface (green circle).

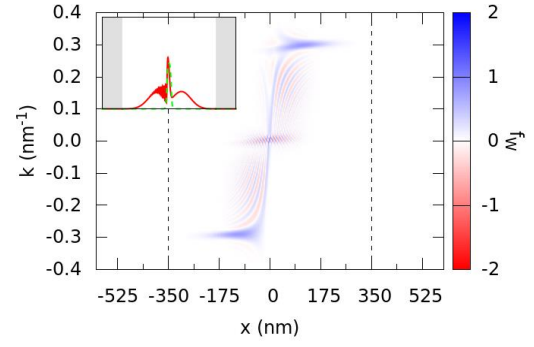


Fig. 6: Wigner distribution function during the scattering at the potential barrier. The inset shows the wave packet (red solid line) scattered by the potential barrier (green dashed line).

On the Consistency of the Stationary Wigner Equation

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The Wigner equation describing stationary quantum transport has a singularity at zero momentum ($k=0$). Numerically the singularity is usually dealt with by just avoiding that point in the grid, a method used, e.g. by Frensley [1]. However, results obtained by this method are known to depend strongly on the discretization and meshing parameters. The method can even yield unphysical results.

We believe that the shortcomings of Frensley's method and related numerical methods are due to the improper treatment of the equation at $k=0$. We propose a revised approach. We explicitly include the point $k=0$ in the grid and derive two equations for that point. The first one is an algebraic constraint which ensures that the solution of the Wigner equation has no singularity at $k=0$. The second is a transport equation for $k=0$. The resulting system, which we refer to as the constrained Wigner equation, is overdetermined. These results are in line with the recent analysis in [2].

An important technical tool is the sigma equation which is the von Neumann equation in a rotated coordinate system. The constrained Wigner equation can be related to a sigma equation with inflow boundary conditions in the spatial coordinate and fully homogeneous boundary conditions in the other coordinate. With these boundary conditions the sigma equation is overdetermined as well. The numerical solution from Frensley's method is related to a sigma equation with anti-periodic boundary conditions in the non-spatial coordinate.

In a single spatial dimension the constrained Wigner and sigma equation have been prototyped. Results fit well with results from the quantum transmitting boundary method.

Acknowledgments. The financial support by the Austrian Federal Ministry of Science, Research and Economy, and the National Foundation for Research, Technology and Development is gratefully acknowledged.

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$$\begin{aligned}\frac{\partial f(r, k)}{\partial r} &= \frac{1}{k} \frac{m}{\hbar} \int f(r, k - k') V_w(r, k') dk' \quad (k \neq 0) \\ \frac{\partial f(r, 0)}{\partial r} &= -\frac{m}{\hbar} \int f_k(r, k') V_w(r, k') dk' \quad (k = 0) \\ \int f(r, k') V_w(r, k') dk' &= 0 \quad (\text{regularity constraint})\end{aligned}$$

Fig. 1: Set of equations referred to as the constrained Wigner equation.

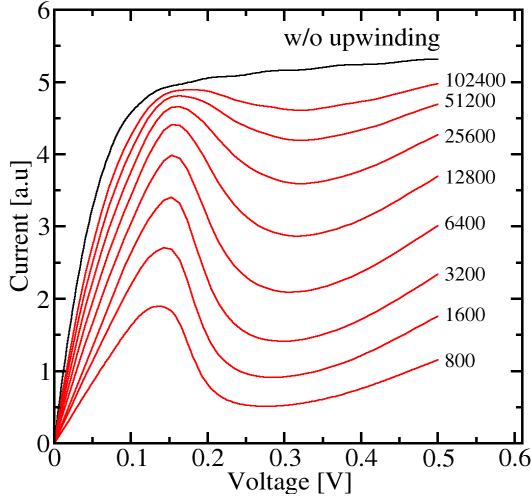


Fig. 2: Breakdown of Frensley's Method. The upper black line is the numerical solution of the unconstrained sigma equation (anti-periodic BCs) without upwinding. The red lines are I-V curves obtained with Frensley's discretization using upwinding. The grid is refined from $N_x=800$ up to $N_x=102400$.

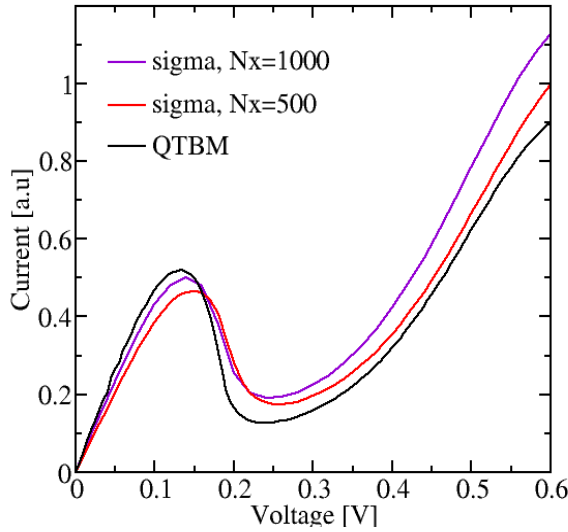


Fig. 3: The numerical solutions of the constrained sigma equation change with grid refinement, but they are quite stable. The resonance from the quantum transmitting boundary method (QTBM) is reproduced.

Posedness of Stationary Wigner Equation

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The problem about the existence and uniqueness of the Wigner equation solution is directly related to physical and computational aspects of actual quantum transport problems. In the case of evolution problems in presence of initial and boundary conditions, it can be shown that there is a unique solution. However, if we consider the long time limit, giving rise to a stationary Wigner picture, it appears that the equation becomes ill-defined: This is associated to the loss of the time derivative and thus the specific evolution role played by the equation in the set of notions needed to define a phase space quantum mechanics. The Weyl map defines an isomorphism from the algebra of the position and the momentum operators \hat{x}, \hat{y} with a product and a commutator $[.,.]_c$ to the algebra of the phase space functions $A(x, p)$ with a non-commutative star $(*)$ -product and Moyal bracket $[.,.]_M$. In particular the evolution of the density operator, the von Neumann equation involving the commutator with the Hamiltonian, gives rise via the Moyal bracket to the equation for the Wigner function. The latter carries the information about the evolution of the physical system, but is not sufficient to define independently phase space quantum mechanics: The $*$ -product is needed to determine the eigenfunctions to provide a physically admissible initial condition. It has been shown that the Wigner equation in presence of the initial and boundary conditions is well posed, i.e. it has a solution which is unique [1]. The proof is based on the resolvent expansion of the integral form of the equation:

$$f(x, k, t) = \int_0^t dt' \int dk' V_w(x(t'), k(t') - k') f(x(t'), k', t) + f_0(x, k) \quad (1)$$

with $f_0 = f_i(x(0), k(0))\theta_\Omega(x(0)) + f_b(x(t_b), k(t_b))\theta_\Omega(t_b)$ and the field-less Newton trajectories $x(t') = x - v(k)(t - t')$, $k(t') = k$ initialized by x, k, t determine the time crossing the boundary, the time t_b by moving backwards in time, $t' < t$ and f_i and f_b provide two complementary contributions from the initial condition and the boundaries. The equation is of Volterra type with respect to the time variable (Markovian evolution) which allows one to prove convergence of the resolvent series under the very general assumption that the potential is absolutely integrable function. The stationary Wigner equation is obtained by the long time limit of (1), using the change $-\tau = t - t'$: $x(\tau) = x + v(k)(\tau)$; $k(\tau) = k$.

$$f(x, k) = \int_{-t=-\infty}^0 dt' \int dk' V_w(x(\tau), k(t') - k') f(x(\tau), k') + f_b(x(\tau_b), k) \quad (2)$$

$-\infty < \tau_b < 0$ is now the time for a trajectory initialized by point x at time 0 to reach the boundary moving backwards.

The limit $f(x, k) = \lim_{t' \rightarrow \infty} f(x, k, t') = \lim_{t \rightarrow \infty} f(x, k, t + \tau)$ defines the stationary solution. Without loss of generality we assumed that the initial condition vanishes in the long time limit. Now we analyze if the existence of the free term f_b in (2) guarantees an unique solution. Or if we formally write the equation as: $(I - \hat{V}_w)f = f_b$, we need to show that the operator $I - \hat{V}_w$ has an inverse operator. This is equivalent to showing that the only solution of the homogeneous equation (2) is the function $f = 0$. We consider the Fourier transform $\tilde{f}(q, k) = 1/2\pi \int dx e^{-iqx} f(x, k)$ and use the change $y = x + v(k)\tau$ to obtain:

$$\tilde{f}(q, k) = \frac{1}{2\pi} \int_{-\infty}^0 d\tau \int dy e^{-iqy} e^{-iqv(k)\tau} \int dk' V_w(y, k') f(y, k - k') \quad (4)$$

The time integral of the exponent can be evaluated in terms of generalized functions to finally give:

$$\hbar q v(k) \tilde{f}(q, k) = \int dq'' \tilde{V}(q'') \left(\tilde{f}\left(q - q'', k + \frac{q''}{2}\right) - \tilde{f}\left(q - q'', k - \frac{q''}{2}\right) \right) \quad (5)$$

with $\tilde{V}(q) = 1/2\pi \int dy e^{-iqy} V(y)$. This equation must be analyzed for existence of non-trivial solutions. Such solutions can be constructed from the stationary Schrödinger equation in momentum space,

$$(E - \epsilon(k))\psi(k) = \int dq \tilde{V}(q)\psi(k - q); \quad \epsilon(k) = \frac{\hbar^2 k^2}{2m} \quad (6)$$

As observed by Carruthers et al. [2] in their study of quantum collisions, the function $f(q, k) = \psi^*(k - q/2) \psi(k + q/2)$ is a solution of (5). Hence the null space of the operator $I - \hat{V}_w$ contains any stationary solution obtained by (6) and we cannot expect a unique solution corresponding to given boundary conditions. This is in accordance with the results presented in [3].

We associate this problem with the loss of the evolution character of the equation: For eigenstates of the Hamiltonian the stationary Wigner equation reduces to $v(k) \partial f(x, k) / \partial x = 0$ with a solution $f(x, k) = \psi(k)$ given by an arbitrary function of k . On the contrary, the evolution problem determined by the time derivative

$$v(k) \frac{\partial f}{\partial x} + \frac{\partial f}{\partial t} = \frac{d f(x(t), k, t)}{dt} = 0 \quad (7)$$

has a solution $f(x, k, t) = f(x(0), k, 0)$ so that a correct physical picture can be obtained by a relevant initial condition $f(x(0), k, 0)$ which obeys the uncertainty relations. In conclusion, both the Wigner equation and the * eigenvalue problem are necessary notions of the phase space quantum mechanics. The stationary limit of the former of the former cannot replace the latter and actually lacks physical argumentation.

Acknowledgments: The financial support by the Austrian Science Fund (FWF) through the projects P29406-N30 and P29119-N30, by the Bulgarian National Science Fund (NSF) through the project DN 12/5-2017 and National Scientific Program ICT-SDM-SES, by the Austrian Federal Ministry of Science, Research and Economy, and by the National Foundation for Research, Technology and Development are gratefully acknowledged.

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Recent Progress in Numerical Methods for Many-Body Wigner Quantum Dynamics

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The Wigner function has provided an equivalent and convenient way to render quantum mechanics in phase space. It allows one to express macroscopically measurable quantities, such as currents and heat fluxes, in statistical forms as usually does in classical statistical mechanics, thereby facilitating its applications in nanoelectronics, quantum optics and etc. Distinct from the Schrödinger equation, the most appealing feature of the Wigner equation, which governs the dynamics of the Wigner function, is that it shares many analogies to the classical mechanism and simply reduces to the classical counterpart when the reduced Planck constant vanishes. Despite the theoretical advantages, numerical resolutions for the Wigner equation is notoriously difficult and remains one of the most challenging problems in computational physics, mainly because of the high dimensionality and nonlocal pseudo-differential operator. On one hand, the commonly used finite difference methods fail to capture the highly oscillatory structure accurately. On the other hand, all existing stochastic algorithms, including the affinity-based Wigner Monte Carlo and signed particle Wigner Monte Carlo methods, have been confined to at most 4D phase space. Few results have been reported for higher dimensional simulations. My group has made substantial progress in both aspects.

(1) We completed the design and implementation of a highly accurate numerical scheme for the Wigner quantum dynamics in 4-D phase space. Our algorithm combines an efficient conservative semi-Lagrangian scheme in the temporal-spatial space with an accurate spectral element method in the momentum space. This accurate Wigner solver has been successfully applied into the investigation of quantum tunneling in double well and quantum double slit interference. Moreover, the Wigner function for a one-dimensional Helium-like system was clearly shown for the first time.

(2) We explored the inherent relation between the Wigner equation and a stochastic branching random walk model. With an auxiliary function, we can cast the Wigner equation into a renewal-type integral equation and prove that its solution is equivalent to the first moment of a stochastic branching random walk. The accuracy of the resulting implementation can be systematically improved and is hardly affected by the choice of time step. In order to further gain a substantial reduction in variances, we propose an asymptotical approach which may ameliorate the sign problem. The performance of 6-D and higher-dimensional simulations demonstrate the accuracy and the efficiency of our asymptotical approach.

It should be noted that all proposed numerical schemes fully exploit the mathematical structure

of the Wigner equation. Our target is an efficient simulator for analyzing some fundamental issues in many-body quantum mechanics, such as the nuclear quantum effect and dynamical correlation.

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Third-Order Correlation Functions of Non-Markovian Quasiprobabilities

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The order of operators detected in quantum weak measurement depends on the measurement setup. This corresponds to different quasiprobabilities, in which a markovian (memory-less) scheme corresponds to the generalized Wigner function and memory effect lead to generalizations [1]. In second order and using a Hamiltonian approach, these different orders are traced back to symmetrized correlators $\sim \langle \{A, B\} \rangle$ and Kubo-type responses $\sim \langle [A, B] \rangle$. [2] The latter terms originate from a so-called system-mediated detector-detector interaction and is intimately related to detectors having a non-zero internal memory time.

Here, we combine the phenomenological proposal for nonsymmetrized correlations in quantum noninvasive measurements and the microscopic derivation of the system-mediated detector-detector interaction of second order to investigate higher-order correlations of non-Markovian weak quantum measurements. The general third-order correlator is introduced in the time domain. We identify and discuss the underlying physical processes before we provide the complete correlation function in the frequency domain, which is the relevant quantity in many experiments carried out e.g. in the measurement of current fluctuations. We find a more complex behavior than in second-order correlations with four types of system operator orders which we denote third cumulant, noise susceptibility I and II and second-order susceptibility, see Fig. 1. We introduce a convenient diagrammatic description which we illustrate by an example of measuring the third-order current correlations of the tunnel current through a barrier.

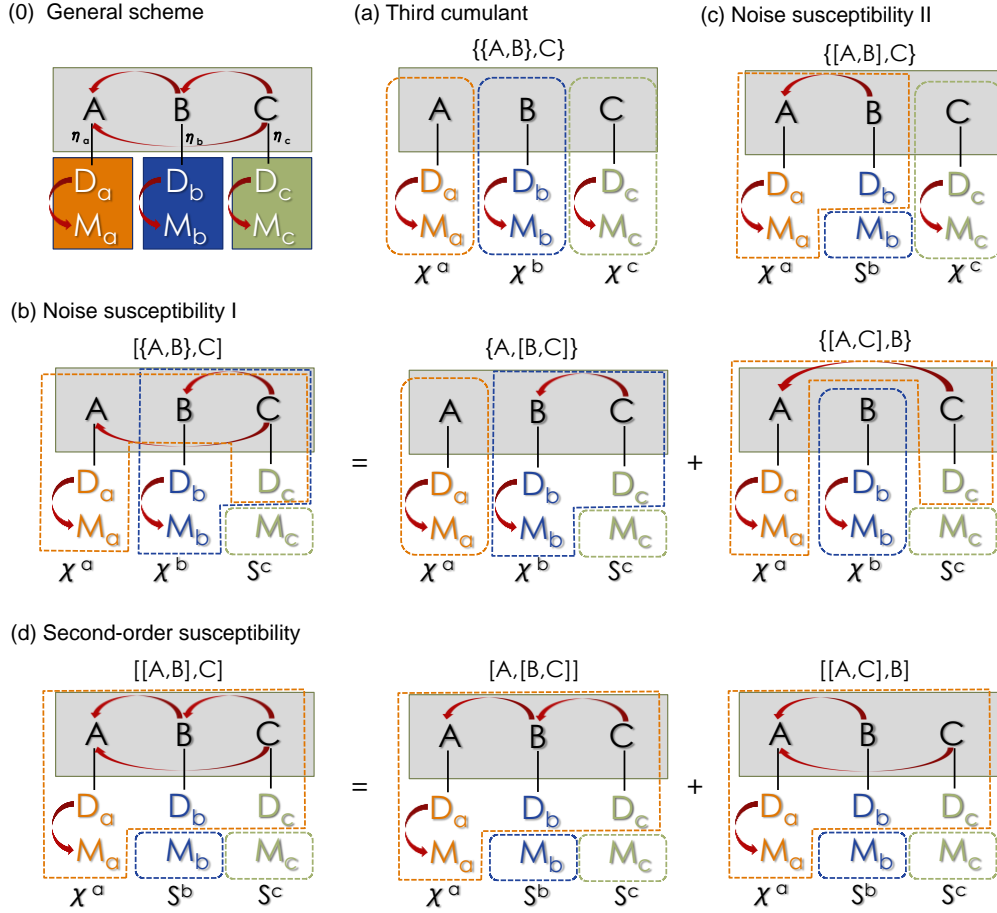


Fig. 1: Correlations of the measured system operators \hat{A} , \hat{B} and \hat{C} in a third-order measurement with the times $a > b > c$. (0) Overview of the interactions. The detector variables that are coupled to the system are denoted with \hat{D}_a, \hat{D}_b , and \hat{D}_c . The red arrows indicate response functions within a subsystem which act only forward in time. The black lines indicate the weak coupling between system and detectors of strength. The occurring third-order correlation are depicted in (a) - (d) and will be discussed in the talk. The dashed boxes frame the paths which are connected to the three measured output variables of the detectors \hat{M}_a, \hat{M}_b , and \hat{M}_c .

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Spin Entanglement in Transition Metal Di-Chalcogenides

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In the transition-metal di-chalcogenides, it is known that, in the presence of the spin-orbit interaction, the doubly degenerate conduction band minima and the valence band maxima are split. In this, the pseudo-spin valley of the two valleys couples to the electron spin to produce a reversal of the normal band spin-splitting at the two degenerate extrema K and K' points [1]. We have earlier reported that this leads to a 2×2 tensor form of the Wigner function for the pseudo-spins of the carriers. In the absence of an electric field, all four elements of the tensor are equivalent. However, when an electric field is applied, the opposite spin-splitting of the two valleys (we deal with the conduction band) leads to a Berry curvature [2] which induces the two spins to move to opposite sides of the sample and leads to a spin Hall effect. In this situation, the off-diagonal elements of the Wigner function develop an oscillatory behavior reflecting the entanglement of the two carriers. In the absence of knowledge about the detailed physics of the sample, the carriers must be defined via a Bohm-type singlet wave function. This entanglement can possibly be used in EPR-type of on-chip devices for spin processing.

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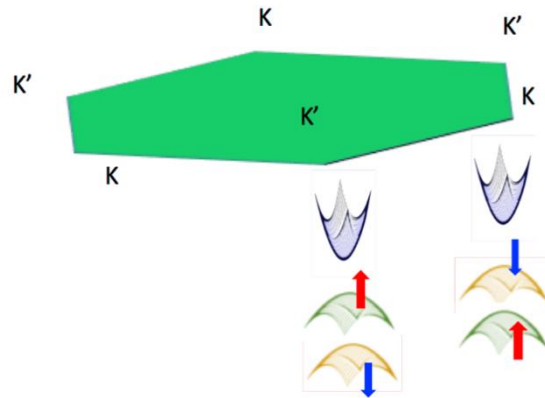


Fig.1: Brillouin zone and energy minima, showing how the spin-splitting is reversed between adjacent minimum points..

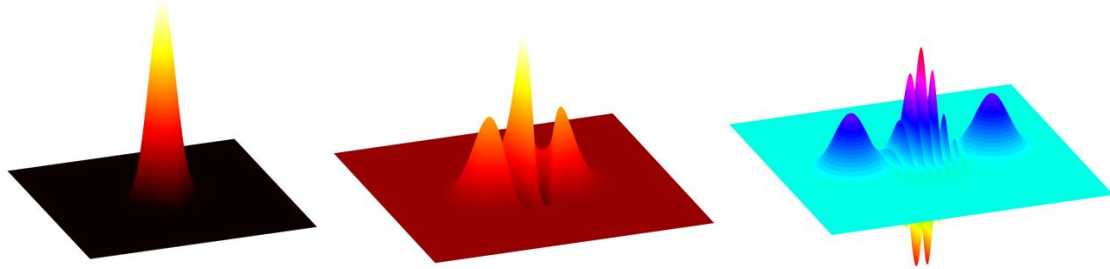


Fig. 2: The total of the four terms of the Wigner function at three various (arbitrary) times. On the left is the joint Wigner function at the initial time the field is applied. At the center is a later time where the two diagonal terms have moved apart and the central peak arises from the sum of the two diagonal terms (which are complex conjugates). At the right, the two diagonal terms have moved further apart and the entanglement is fully formed and evident (the second time is twice that of the center image). The color schemes are actually similar, and the blue of the right panel indicates the decrease in amplitude of the Wigner functions at this later time—the peak in the left panel is some 4 times the separated peaks in the right panel.

Formulation of a Complex Absorbing Potential for the Transient Numerical Solution of the Wigner Transport Equation

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Along with the numerical solution of the Wigner Transport Equation (WTE) several numerical difficulties arise [1]. Conventional finite difference approaches applied onto the WTE are based on so-called upwind difference schemes (UDS) [2] leading to an inadequate inclusion of coherent effects [1]. As a result, the diffusion effects are overestimated [3]. In addition, the inflow boundary conditions are not linked with the drift operator contradicting the non-local character of quantum mechanics [1]. As a consequence, the numerical solution of the WTE suffers from inherent errors. To overcome these limitations an approach based on the formulation of an exponential operator (EO) has been proposed recently [1].

When deriving the classical WTE in center-mass coordinates, χ and ξ [2], it is conventionally presumed that an additional term arising from the partial integration of the diffusion operator in real space is equal to zero. This particular term is related to the boundary values of the statistical density matrix with respect to the ξ -direction. For the corresponding analytical investigations, an infinite computational domain is presumed, but for numerical calculations a finite computational domain has to be supposed. Hence, the omission of this term leads to conceptual errors imposing Dirichlet boundary conditions according to a zero valued statistical density matrix. Unfortunately, no analytical expression or approximation can be derived for this term, which can be incorporated within the algorithm for the numerical solution of the WTE.

To overcome these limitations, an approach based on the formulation of a complex absorbing potential is proposed for the numerical solution of the WTE, which is already utilized in a similar manner for the numerical solution of the Schrödinger equation [4]. The main idea behind the approach is the introduction of a local absorber within the real space, which prevents artificial reflections caused by the finiteness of the computational domain with respect to the ξ -direction due to the Dirichlet boundary conditions. Within the local absorbers an additional damping term is present leading to a decaying statistical density to a negligible value close to zero near the boundary. As a consequence, conceptual errors can be effectively avoided, because the omission of the boundary term is now justified.

The approach is validated by means of a simply structured resonant tunneling diode. From the results obtained, it can be concluded that the complex absorbing potential offers major improvements with regard to the numerical solution of the WTE.

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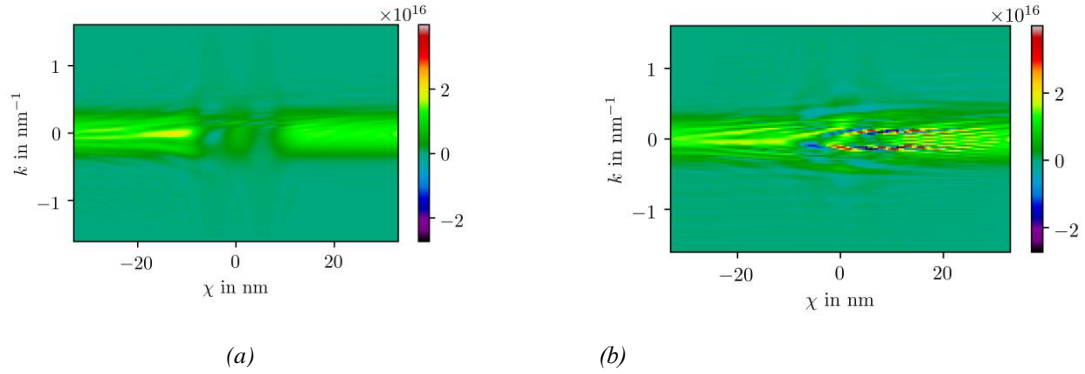


Fig.1: Wigner functions for the resonant tunneling diode in the transient non-equilibrium situation with an applied external bias after 2500fs. The resonant tunneling diode is initially in the thermal equilibrium state. At the time $t=0$ fs a constant bias according to -0.11 V is applied driving the device into a non-equilibrium state. The time evolution of the Wigner function utilizing the complex absorbing potential is shown in (a), whereas the classical solution of the WTE is shown in (b). A Low-Storage-Runge-Kutta scheme of 4th order approximates the time domain propagator. In comparison, an artificial interference pattern caused by the inadequate inclusion of the boundaries with regard to the ξ -direction can be observed from (b). Along with the application of the complex absorbing potential this unphysical interference pattern can be effectively avoided as can be seen from (a).

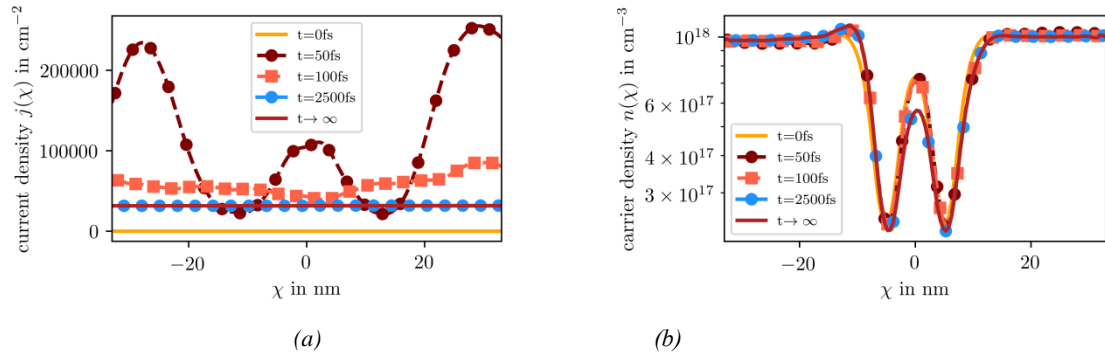


Fig.2: Transient evolution of the current density j depicted in (a) and of the carrier density shown in (b) for the biased resonant tunneling diode, which are calculated from the corresponding Wigner functions. In addition, the stationary solutions are shown ($t \rightarrow \infty$). As can be observed, the current density as well as the carrier density converge exactly towards the stationary reference solution.

Accuracy Balancing for the Discrete Wigner Transport Equation Adopting Higher-Order Differencing Schemes

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The Wigner function $f(q,k)$ is defined on phase space. Two actions in orthogonal directions of the phase space, diffusion in q space and transition in k space, are described by the Wigner transport equation (WTE) with its kinetic and potential terms [1]. For the finite-difference-based analysis of the WTE, we have to introduce two numerical parameters Δ_q and Δ_k (mesh spacings in phase space). A smaller Δ_q (Δ_k) enhances the numerical accuracy of the kinetic (potential) term [2,3]. Δ_k cannot be made smaller than π/L where L denotes the device length [4], setting the maximum degree of numerical accuracy of the potential term. With this fixed degree of numerical accuracy of the potential term, increasing indefinitely the degree of numerical accuracy of the kinetic term leads to unphysical simulation results [2,3]. To avoid them, we need to seek a balance between these two degrees of numerical accuracy. That is, we cannot pursue a satisfactorily high accuracy in solving the finite-difference-based or discrete WTE. Instead, we have to be satisfied with an optimum solution.

The kinetic term of the WTE is proportional to the differentiation of $f(q,k)$ with respect to q . There are several differencing schemes (DSs) developed for this differentiation. In [2,3], we have found the optimum solution of the discrete WTE with the first-order DS (FDS) from the perspective of accuracy balancing. However, it is probable that the use of higher-order DSs such as the second-order DS (SDS) and the third-order DS (TDS) results in different optimum solutions. In this work, we demonstrate that in the simulation of resonant tunneling diodes (RTDs; see Fig. 1), we cannot find appropriate optimum solutions with SDS (Figs. 2 and 3) or TDS (Figs. 4 and 5), in contrast to a converging optimum solution obtained with FDS (Fig. 6) [2]. This poses the possibility that higher-order DSs are not always a better option than the FDS.

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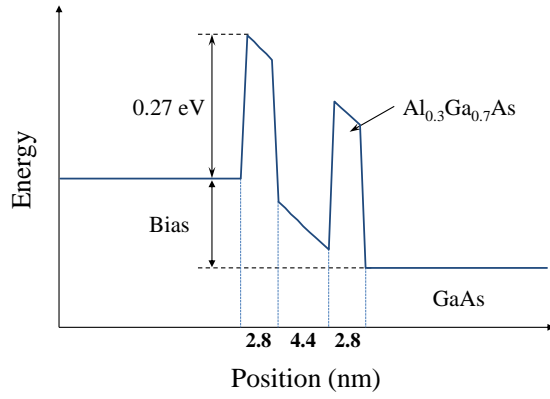


Fig. 1: The RTD model used in the simulation.

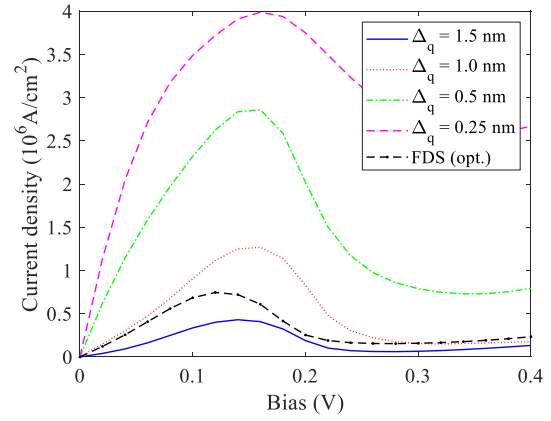


Fig. 4: I - V characteristics of the RTD with TDS and $\Delta_k = \Delta_{k0}$.

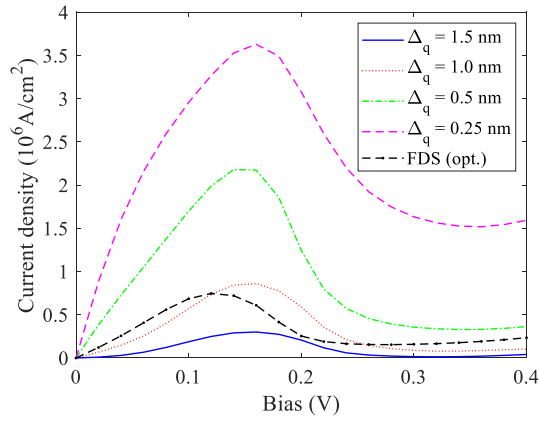


Fig. 2: I - V characteristics of the RTD with SDS and $\Delta_k = \Delta_{k0} = 0.067 \text{ nm}^{-1}$. The optimum result with FDS ($\Delta_q = \Delta_{q0} = 0.25 \text{ nm}$) is also shown for comparison.

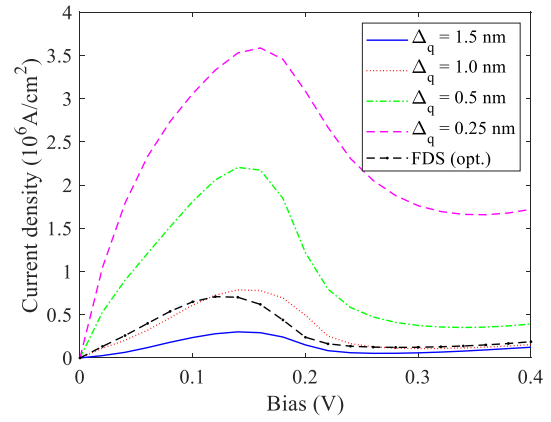


Fig. 5: The same as Fig. 4 with $\Delta_k = \Delta_{k0}/2$.

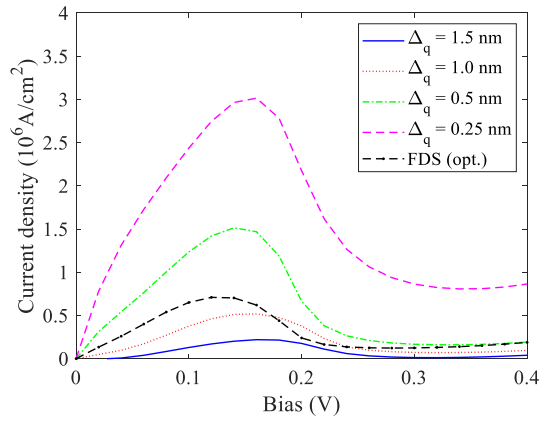


Fig. 3: The same as Fig. 2 with $\Delta_k = \Delta_{k0}/2$. The optimum result with FDS ($\Delta_q = \Delta_{q0}/2$) is also shown.

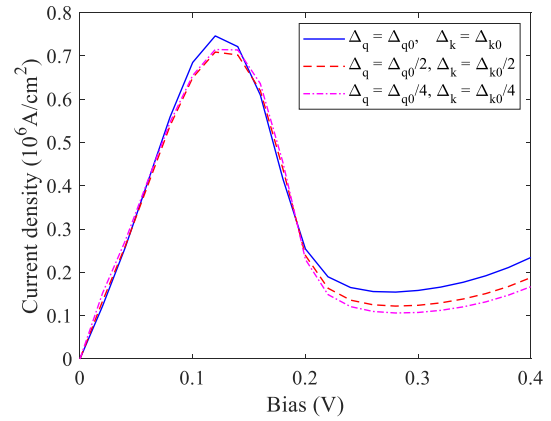


Fig. 6: Optimum results with FDS. They converge with decreasing Δ_k . This characteristic cannot be observed with SDS and TDS.

