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IW^2 2017

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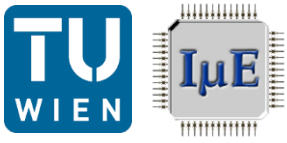

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Welcome to the **Second International Wigner Workshop (IW^2)**. The workshop is a one day meeting and brings together researchers from all areas of science and engineering, areas in which Wigner functions have been or could be applied. The 2017 Workshop marks the second installment of this series (the first was held in Hawaii, in December, 2015) 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 were reviewed by the 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 ten invited speakers and accepted eleven regular speakers as well as five poster presentations.

We would like to express our gratitude to our sponsors (in particular the *United States Office of Naval Research Global* and the *Institute of Physics*) 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 the Lake District.

David K. Ferry and Josef Weinbub
Chairs of IW2 2017
May, 2017

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Program

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13:50-14:20	**Cavity QED of Atoms: Cooling, Trapping and Many-Body Physics** Peter Domokos (invited)	**20**
14:20-14:40	**Transport Properties of Quasiperiodic Systems** Maciej Wołoszyn	**22**

Wigner Function Representation in Electron Quantum Optics

Dario Ferraro[1]

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I will investigate various aspects of the new and fast developing field of the electron quantum optics [1], namely the possibility to realize optics-like experiments with individual electrons (or holes) propagating along integer quantum Hall edge channels. Differently form what happens for the photonic counterpart, in the electronic case the effects of Fermi statistic and Coulomb interaction have to be properly taken into account and strongly affect the physics. I will consider a time-frequency description of the electron first order coherence (two point Green's function) in analogy with the Wigner function representation in quantum mechanics [2]. This approach reveals extremely useful in order to characterize, in terms of a unique real function, both the coherence properties in the time domain and the nature of the excitations generated by single or few electron sources realized by various experimental group. Recently a reconstruction of the Wigner function through tomographic measurements has been presented according to the present theoretical discussion [3].
When individual electron sources are used as inputs of a Mach-Zehnder interferometer, the quantum interferences emerge in a clear way in this mixed representation. I will discuss the evolution of the mean current as a function of time as well as the energy spectrum, which are affected in a complementary way by the interference. These quantities are the marginal distributions associated to the Wigner function. The above description revealed very useful in order to provide a compact and clear description also for two-electrons interferometry experiments analogous to the Hanbury-Brown-Twiss [4] and the Hong-Ou-Mandel [5] in quantum optics and to develop efficient tomographic protocols.
In terms of this representation it is also easy to visualize both in the time and the energy domains the effects of the interaction with the external environment, its role in leading to decoherence and relaxation of the injected electronic wave-packet and consequently the robustness of the output of the various possible electronic sources [6]. In particular, the Landau excitation (Lorentzian wave-packet in energy generated by a single electron source) exhibits a fast relaxation followed by spin-charge separation whereas the Levitov excitation (Lorentzian wave-packet in time generated by a well designed voltage pulse) only experiences spin-charge separation. An essential theoretical tool to deal with the interacting case is represented by the scattering matrix acting on the edge-magnetoplasmons, relevant degrees of freedom of the edge channels in presence of interaction with an external linear environment.

This research has been supported by the Franch National Grants "1 shot" (ANR-2010-BLANC-0412) and "1 shot reloaded" (ANR-14-CE32-0017).

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Squeezing of Optical Phonons Generated by Different Optical Excitations of a Quantum Dot: A Wigner Function Analysis

Daniel Wigger[1], Helge Gehring[1], V. Martin Axt[2], Doris E. Reiter[1], and Tilmann Kuhn[1]

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The study of the fundamental properties of phonons is crucial to understand their role in applications in quantum information science, where the active use of phonons is currently of high interest. We are studying the interplay of single excitons in optically driven semiconductor quantum dots (QDs) and the crystal lattice. In this contribution we concentrate on the coupling to optical phonons. For the phonon wave vectors that are coupled to the exciton the dispersion is rather flat and can be modelled by a constant energy. This allows us to transform the exciton-phonon coupling from a multimode case to just a single coupled longitudinal optical (LO) mode. A schematic picture of the coupled exciton-phonon system is shown in Fig. 1(a). The phonon can either be in the potential of the exciton ground state $|g\rangle$ or the exciton state $|x\rangle$. These two harmonic confinement potentials of the phonons are shifted with respect to each other by twice the exciton-phonon coupling strength Γ. For the single mode the representation of the phonon quantum states in form of Wigner functions provides a very intuitive way to study their properties.

The aim of this study is to find laser pulse excitation schemes of the QD exciton that result in squeezed phonon states. A squeezed state is characterized by fluctuations of one variable, lattice displacement U or momentum Π, that fall below the respective vacuum value.

In the limiting case of an excitation with ultrafast laser pulses, which we model by δ-functions, every excitation leads to the creation of a coherent state in the phonon system because of the displaced equilibrium position. Depending on the pulse area of the laser pulse, part of the phonon state, can however, remain in the excitonic ground state. The complete quantum state of the coupled system is hence an entangled exciton-phonon state. When tracing over the excitonic degrees of freedom, the phonon state reduces to a statistical mixture of the vacuum state and a coherent state. It is obvious that after such an ultrafast excitation, no squeezing can occur. But it turns out that for a sequence of two ultrafast pulses, a superposition of two coherent states in each excitonic subsystem is created. Consequently, for the phonons a statistical mixture of two Schödinger cat states builds up. The dynamics of the LO phonon Wigner function is given in Fig. 1(b), where the two dumbbell structures are visible being characteristic for cat states.

Each dumbbell rotates around a different point in phase space according to the two different equilibrium positions. The calculations are performed for an artificially increased coupling strength Γ. For realistic values of Γ, the different parts of the Wigner function overlap and squeezing can occur [1].

In a second step we discuss the phonon properties for an excitation with finite pulses. Within a generating function formalism, we calculate the corresponding Wigner functions numerically. Here even for a single-pulse excitation squeezing can occur. The Wigner function for an intermediate pulse duration is shown in Fig.1(c). In each excitonic subsystem (W_g and W_x) we find a superposition of the two phonon Fock states $|0\rangle$ and $|1\rangle$ [2].

We show that the two previously introduced excitation schemes, namely (i) the superposition of two coherent states for two ultrafast excitations, and (ii) the superposition of two Fock states for extended single pulse excitations, can lead to squeezed LO phonons.

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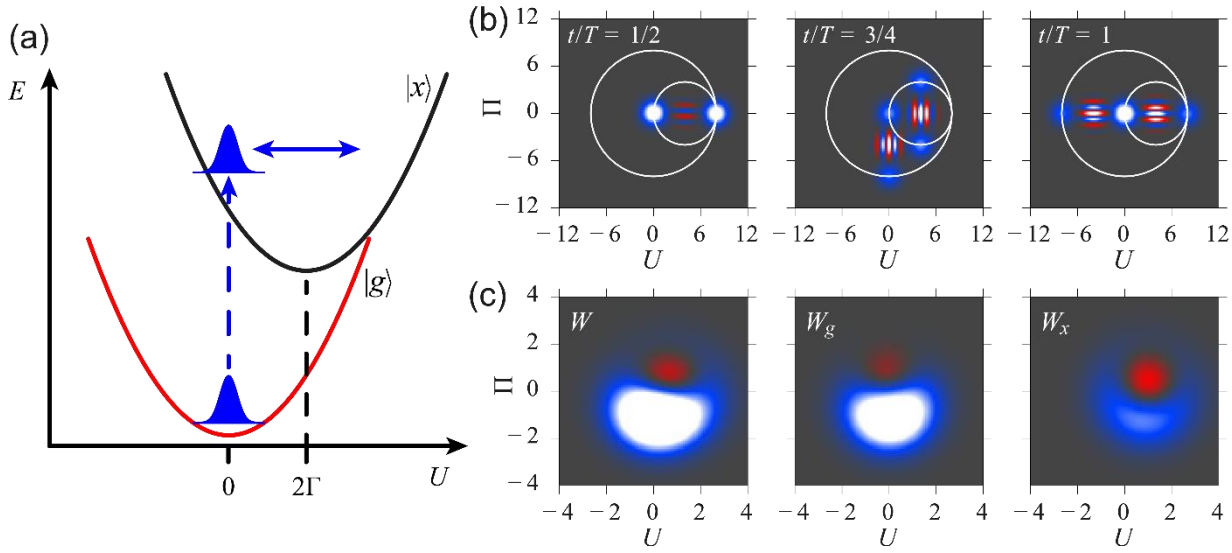

Fig. 1: (a) Schematic picture of the coupled exciton-phonon system. (b) Phonon Wigner function after the excitation with two ultrashort pulses. (c) Phonon Wigner function after the excitation with a single laser pulse with intermediate duration.

Full Reconstruction of Symmetric Two-Mode Optical Quantum States with Gaussian Wigner Function via Spectral Homodyne Detection

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Gaussian states are quantum states with Gaussian Wigner functions and, thus, are fully characterized by their covariance matrix and first moment vector. In the optical domain, states belonging to this class, as vacuum, coherent, squeezed and thermal states (see Fig. 1), play a central role not only in quantum information with continuous variable [1,2] but also in high-precision quantum interferometry [3,4], since they can be generated and manipulated by current technology. Moreover, optical Gaussian states can be engineered to create non-Gaussian states still useful to quantum information processing, such as single photon states or polarization entangled two-photon states [5].
Here we briefly review of the basic concepts and mathematical tools needed for phase-space description of Gaussian states, focusing on their manipulation through symplectic transformations and propagation also in the presence of losses. Then we discuss our recent theoretical and experimental results obtained about the full characterization of symmetric two-mode squeezed thermal states via spectral homodyne detection and a state-balancing detector [6]. More precisely, we address the characterization of the signal from an optical parametric oscillator (OPO), that is the main source of continuous-variable quantum states exploited in quantum-information processing protocols.
Homodyne detection is an effective tool to characterize the quantum state of light in a narrow spectral range. We demonstrate that the relevant information for the quantum state reconstruction of the symmetric spectral modes is obtained by using both a single homodyne detector and the error signal from the active stabilization of the oscillator cavity (see the left panel of Fig. 2). The latter is based on the Pound-Drever-Hall technique [7]. The error signal from the PDH is used to stabilize the OPO as well as to monitor the state balance. The reconstruction is achieved by exploiting the phase coherence of the setup, guaranteed in every step of the experiment, and two auxiliary combinations of the sideband modes selected by suitably setting the mixer phases (see the right panel of Fig. 2). The measurement scheme has been successfully tested on different states, ranging from uncorrelated coherent states to entangled states generated by two-mode squeezing. Our procedure is indeed a versatile diagnostic tool, suitable to be embedded in quantum information experiments with continuous variable systems in the spectral domain.

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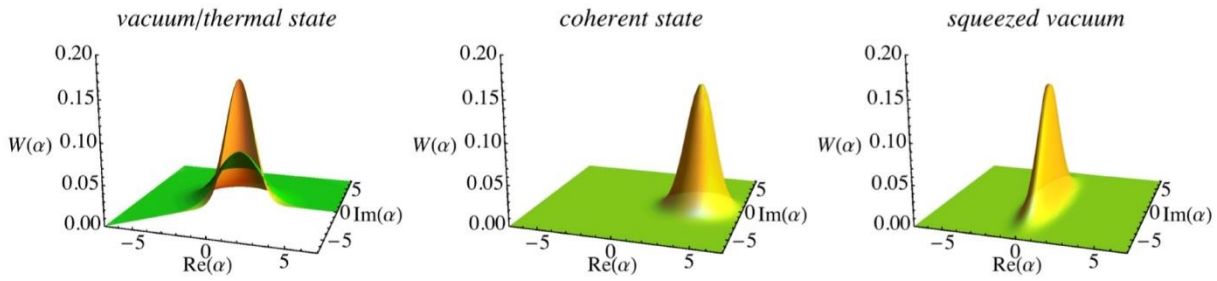

Fig. 1: Gaussian Wigner functions of the vacuum state (left plot, yellow) and of a thermal state (left plot, green), of a coherent state (center) and of a squeezed vacuum state (right). Note that, though the squeezed vacuum state is non-classical, its Wigner function if positive.

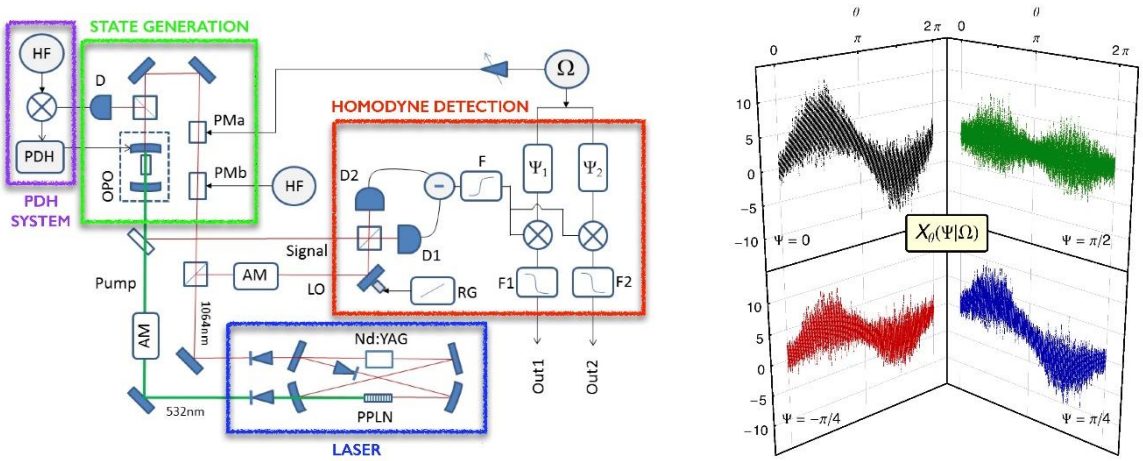

Fig. 2: (Left) Schematic diagram of the experimental setup for the generation and reconstruction of symmetric two-mode Gaussian states from an OPO. (Right) Examples of the homodyne traces used for reconstruction of the signal (here a squeezed-coherent two-mode sideband state). Scheme and data from Ref. [6].

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On Wigner Functions in Dirac-Like Bands: The Transition Metal Di-Chalcogenides

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It is well-known that the Wigner function in Dirac bands takes a tensor form due to the spin and energy degeneracies. In recent years, the importance of Dirac-like bands in semiconductors has been recognized beyond the zero-gap graphene case. For example, the introduction of **k•p** perturbation and spin-orbit interaction lead to Dirac-like bands in gapped semiconductors, of which the transition-metal di-chalcogenides provide a particularly interesting case [1]. Here, the lack of inversion symmetry in the monolayer crystal couples to need for time reversal symmetry in the spin splitting to produce a reversal of the normal spin-split valence bands at the two degenerate extrema K and K' points of the Brillouin zone (Fig. 1) [2]. The spin couples to the pseudo-spin of the two valleys, producing a spin-valley interaction that leads to this effect. Since the material is gapped, we need only consider the positive energy solutions, with the pseudo-spin already incorporating the spin separation. As a result, the Wigner tensor can be expressed as a 2×2 tensor in the pseudo-spin, as f_{ij}, where i,j=K, K' refer to the two degenerate conduction band valleys. In the absence of an electric field, all four elements are equat to one another due to the symmetry. However, when an electric field is applied, the opposite spin splitting leads to a Berry curvature [3] $\Omega\sim\tau f$, where τ is the pseudo-spin index (±1) and f is a function of the band structure parameters. This is opposite in the two valleys, causing them to move in opposite directions perpendicular to the electric field, producing a valley Hall splitting (Fig. 2). In this situation, the off-diagonal elements of the Wigner tensor develop an oscillatory behaviour reflecting the entanglement of the two diagonal valley terms. In this talk, we describe the full model for the spin-valley interaction, and compute the four elements of the Wigner tensor, illustrating how the oscillations and the valley Hall splitting arise naturally from the Dirac-like band structure.

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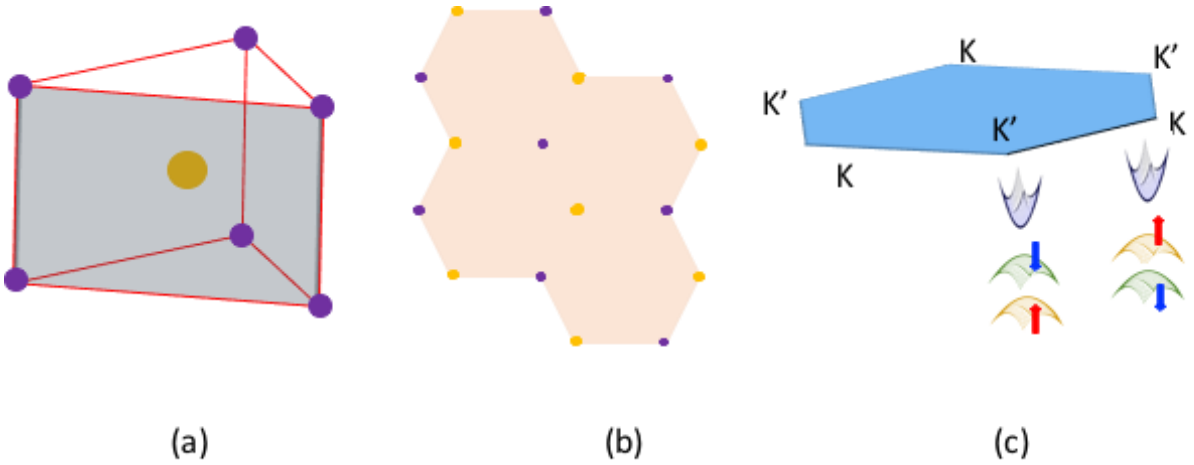

Fig. 1. (a) Lattice structure of the TMDC. The orange atom is the transition metal, while the purple are the chalcogenides. The structure is a tri-layer with metal in the central layer and chalcogenides in the top and bottom layer. (b) Monolayer crystal structure, showing the lack of inversion symmetry. (c) Brillioun zone and energy minimum, showing how the spin splilting is reversed between adjacent minimum points.

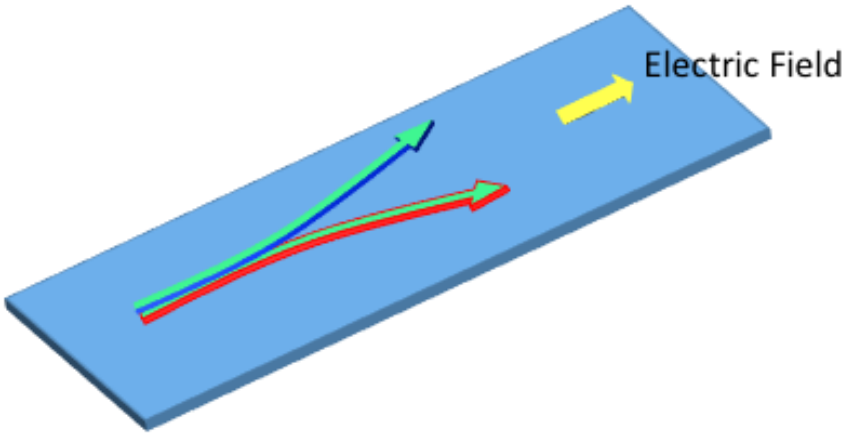

Fig. 2. Illustration of how the two spin reversals lead to motion toward opposite sides in the presence of an electric field. This separation gives a valley-spin Hall effect.

Generalized Phase Space Distributions of Observables in Quantum Transport

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The Wigner function can be considered as general concept of a phase-space distribution of non-commuting variables. In particular, in the field of mesoscopic transport the observables are typically the current operators at a given frequency I_ω, which can be observables similar to position and momentum. The currents are usually measured electronically and it has been shown that in general such weak measurement lead to Keldysh-ordered correlations functions, thus defining a generalized Wigner functional of the time-dependent current [1]. It can be shown that the Wigner functional at a voltage-biased tunnel junction at low temperatures can be negative, which can be tested by violating a classical inequality involving fourth-order current correlators [2]. Since the operator-ordering depends on the measuring setup, alternative measuring scheme involving detectors with memory allow to address generalized normal or anti-normal ordering [3]. This has been experimentally verified by showing a squeezed state in a driven tunnel contact [4]. In this talk I will present an overview of these concepts, relate them to some general properties of the negativity of the Wigner function, and will discuss suggestions for setups to measure the generalized phase space distributions.

This research has been supported by the DFG through SFB 767.

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Challenges in Simulating Dissipative Transport in Nanostructures Using the Wigner Transport Formalism

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There are three major types of difficulties that hinder the widespread use of the Wigner transport formalism in device simulation, despite the formalism's intuitive appeal and the natural framework that it offers for the treatment of transients. These challenges are: 1) increasing computational burden with increasing dimensionality of the structure; 2) the issues arising from inappropriate application of boundary conditions or erroneous electron distributions injected from the contacts in a numerical simulation; and 3) the incompatibilities and tradeoffs that stem from trying to capture both coherent transport features and dissipation. The first challenge is a long-standing one and has been addressed in the coherent transport limit [1,2]. The latter two have been gaining recognition in the community in recent years as critical to the technique's viability [3-8].

In this paper, we address the second and third challenges, with focus on the last one. Namely, the commonly used Boltzmann collision operator in the Wigner transport equation is satisfactory only in systems in which electronic transport is mostly semiclassical (i.e., there is little tunneling) [5]. In systems with pronounced tunneling, such as superlattices or quantum cascade lasers [4,6], the Boltzmann collision operator leads to greatly erroneous results. We discuss the inherent difficulties in developing a Wigner function formalism that would correspond to the completely positive map for the evolution of the accompanying density matrix, which is a requirement needed to ensure physically meaningful results at all times. The dissipative term in the density matrix formalism is derived in the interaction picture, which means that the eigenstates of the unperturbed system are needed to cast the dissipator, but which also somewhat defeats the purpose of using the position-momentum basis that underpins the Wigner function technique. Here, we will discuss recent progress in understanding how to unlock the key strengths of the Wigner approach that apply to open electronic systems in nanostructures when thinking about dissipative transport.

This work has been supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DESC0008712. The work was performed using the resources of the UW-Madison Center for High Throughput Computing (CHTC)

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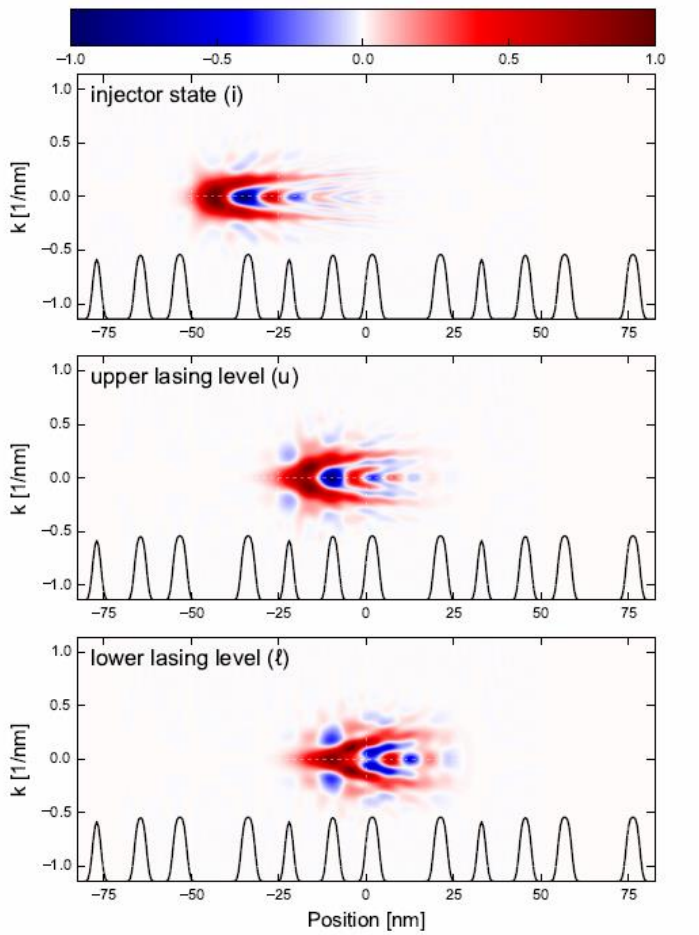

Fig. 1: (Top to bottom) Wigner functions for an injector state (i), the upper lasing level (u), and the lower lasing level (*l*) in a THz quantum cascade laser. Based on Refs. [4,6].

Wigner-Boltzmann Monte Carlo Simulation: From Ballistic to Diffusive Quantum Transport in Semiconductor Devices

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The Wigner description of quantum mechanics is a phase-space formulation of the quantum theory, based on the Wigner function that is both the phase-space counterpart of the density matrix and the quantum counterpart of the classical distribution function. Hence, as the Boltzmann formalism in classical transport, the Wigner formalism provides a powerful framework of quantum transport of particles, suitable for semiconductor device simulation with open-boundary conditions. However, as with all formalisms of quantum transport, beyond the description of coherent transport, the accurate implementation of electron scattering (with phonons or impurities) is an issue from both the physical and the numerical perspectives. For instance, to describe the electron-phonon interaction, it is a priori required to define a generalized Wigner function including the phonon states [1]. After solving the resulting generalized Wigner equation, which is far from trivial, the reduced (electron) Wigner function of interest can be obtained by taking the trace over the phonon modes. To reduce the complexity of this approach, the Wigner-Boltzmann equation (WBE) can be obtained after a hierarchy of approximations, including the weak scattering limit and assuming the phonon system to be in equilibrium, and after taking the classical limit of the phonon term, which leads to the instantaneous and local collision operator [2].

The WBE can be solved using a particle Monte Carlo technique, for instance using the "affinity" [3] or the "signed-particle" [4] method. The results presented here have been obtained using the affinity method that is very convenient for device simulation. Though the WBE was shown to have limitations for large quantum systems as superlattices [5] or if the states generated by the collision operator are not properly chosen [6]. It has been successfully employed to treat many problems of quantum transport. Here, we will review some of them, including phonon-induced decoherence of a wave packet [7] and transport in resonant tunnelling diodes and nanotransistors. They are illustrated in Figs. 1 (decoherence in a RTD), 2 (*I-V* characteristics of a RTD) and 3 (*I-V* characteristics, Boltzmann function and Wigner function of a 6 nm-MOSFET). Finally, we will discuss the potential prospects of this approach.

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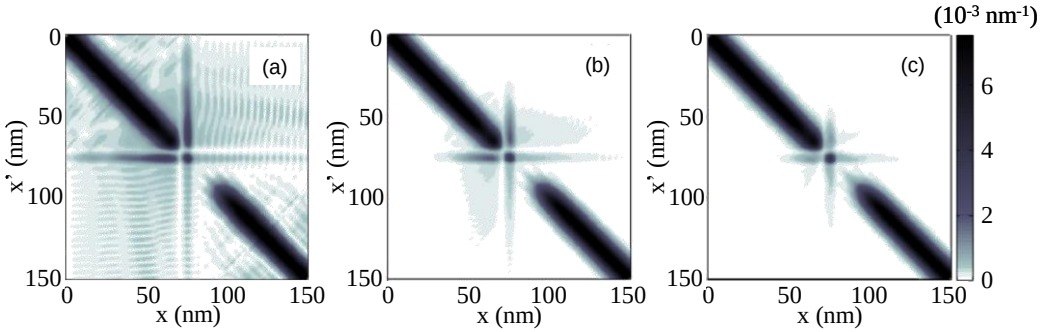

Fig. 1. Density Matrix modulus of the RTD operating at the peak voltage with (a) no scattering, (b) standard scattering rates, and (c) scattering rates multiplied by five.

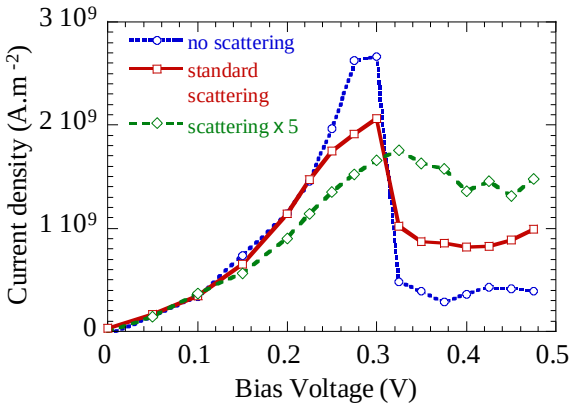

Fig. 2. I-V characteristics of a RTD at 300K with scattering artificially deactivated (circles), with standard scattering rates (squares) and with scattering rates multiplied by 5 (diamonds).

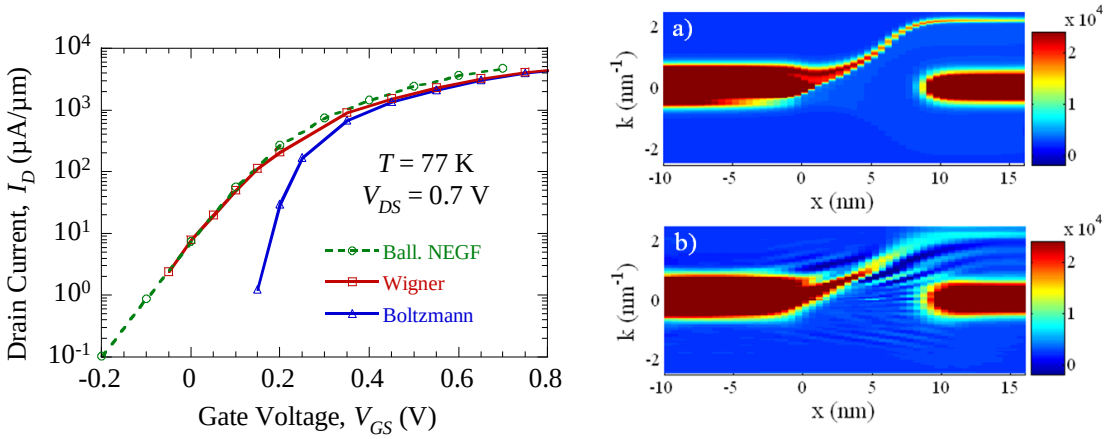

Fig. 3. (right) *I-V* characteristics of (a) 6 nm-DG-MOSFET at T = 77 K using three types of mode-space simulation, (left) Map of (a) semi-classical distribution function and (b) Wigner function of the 1st sub-band of MOSFET at T = 300 K, for V_{GS} = 0.45 V and V_{DS} = 0.7 V.

Potential Problems in the Application of Wigner-Boltzmann Equation in the Time-Dependent Modelling of Dissipative Quantum Transport

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Typically, open systems are modelled through the reduced density matrix or the Wigner distribution function. An equation of motion for the Wigner function (or the density matrix) requires a coherent term plus a collision term that accounts for the interaction of the open system with the environment. The exact shape of this collision term is unknown and reasonable approximations are mandatory. In the Wigner formalism, it is quite common to use the Boltzmann collision operator. The inclusion of such operator into the Liouville equation generates the so-called Wigner-Boltzmann equation. An equation of motion can be interpreted as a dynamical map which has to satisfy some necessary conditions: among them, complete positivity which guarantees that the charge density is positive at any time. *Does the Wigner-Boltzmann equation satisfy complete positivity?* In this conference, we will discuss this issue from numerical simulations.

The effects of the Boltzmann collision operator on the Wigner function can be interpreted as *subtracting* and *adding* parts of the Wigner function. The absorption of a phonon with momentum q by an initial electron with momentum k_o can be understood as *subtracting* the part of the Wigner function representing an initial electron of momentum k_o and *adding* another part representing another electron with final momentum $k_f=k_o+q$. The so-called Wigner-Boltzmann equation of motion cannot guarantee the mentioned completely positivity as can be seen numerically (Fig. 1) where unphysical negative charge density appears [1-3]. This unphysical feature of the Wigner-Boltzmann equation of motion can be solved by knowing which are the states conforming the open system. With such information, the Boltzmann collision operator does not need to be interpreted in terms of subtracting/adding parts of the Wigner function, but in terms of modifying one state from its initial momentum k_0 before the scattering to its final momentum k_f. The knowledge of the states that build the Wigner function (or the density matrix) in an open system with dissipation can be obtained by using numerical techniques dealing with the Bohmian conditional wave functions [4-6]. By construction, positive expectation values of the charge density are always obtained when dealing with such states (Fig. 2).

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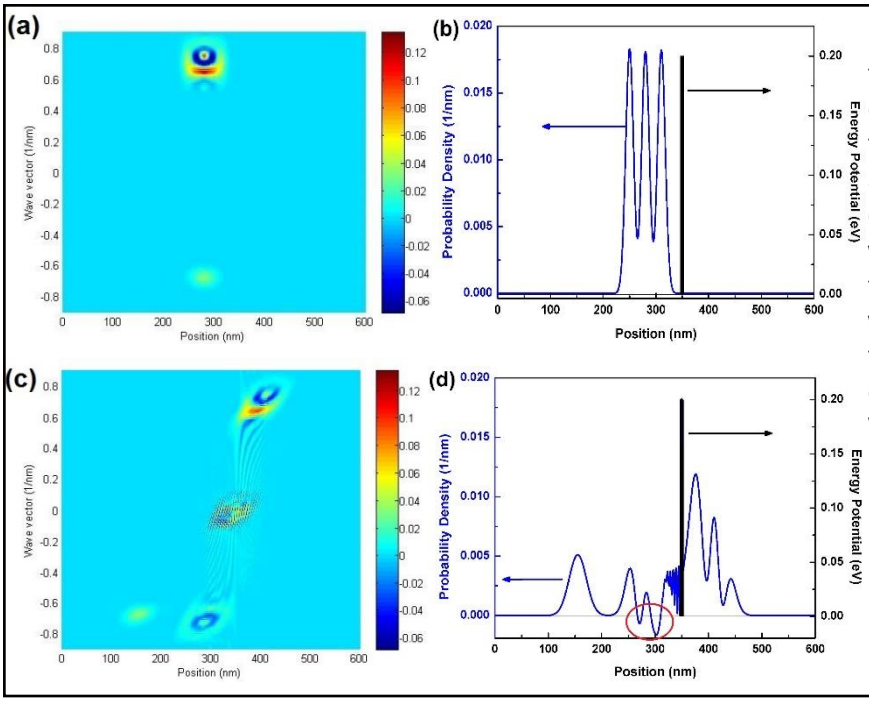

Figure 1. Evolution of the Wigner function of electrons suffering a collision with a phonon while moving towards a double barrier located at 350 nm. (a) and (c) are the Wigner distributions at time t_S=0.006 ps when the scattering occurs and at t_2=0.315 ps when the interaction with barriers occurs. (b) and (d) are the corresponding probability density (momenta integral of the Wigner function). The collision is modelled through the Wigner-Boltzmann equation of motion mentioned in the text. In this model, negative charge density appears in (d) pointed out by the red circle.

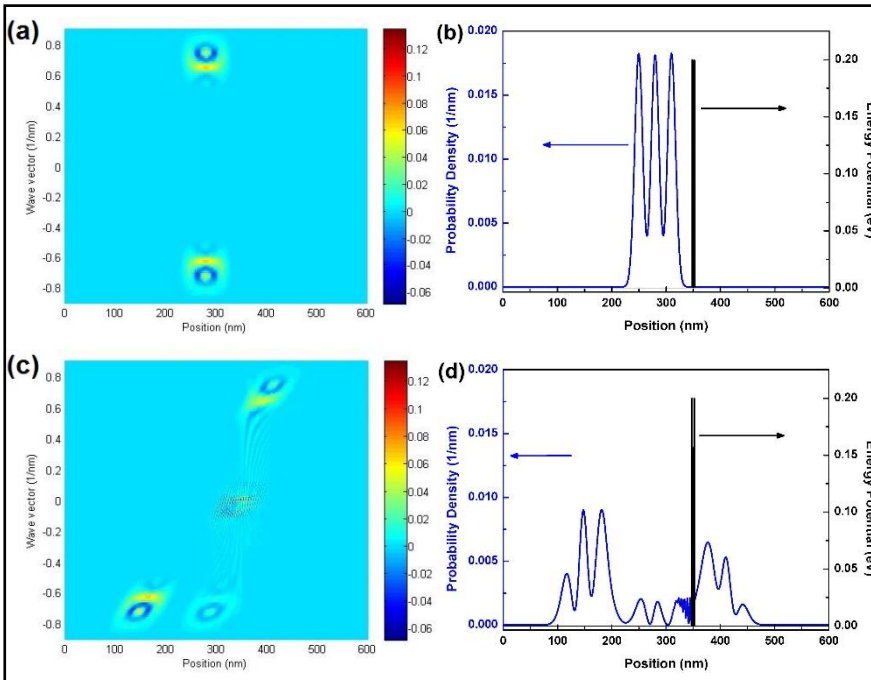

Figure 2. Same simulation as in Fig.1, but treating the collision with the Boltzmann collision operator adopting conditional wave functions. Such scattering process can be interpreted as modifying the states representing Wigner function, which ensures positive charge density at any time.

The simulation parameters in both figures are: wave packet energy E=0.09 eV, effective mass $m^*=0.2m_0$, where m_0 is the free electron mass, the barrier height is 0.2 eV, the barrier width is 0.8 nm and the well width is 4 nm.

Wigner Function and Decoherence

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In the last decades decoherence has stimulated particular interest in theoretical physics, mainly because it constitutes the bridge between quantum and classical physics. Decoherence is strictly related to entanglement: If, e.g., the position coordinate of an electron becomes entangled with a variable of the environment, decoherence appears in the calculation when the trace over the "external" variables is performed in order to obtain the reduced density matrix of the electron.

The Wigner function (WF) has proved to be a useful theoretical concept to study (mainly through its visualization) the phenomenon of decoherence. Since the entanglement between the electron coordinates and the environment occurs during the dynamical evolution of the combined system, first the definition of the WF must be extended to include the environment variables and then traced over such variables to obtain a "reduced WF". This means that the simulation of the WF must be performed to eventually obtain diagonal elements with respect to the environment variables.

Several methods have been devised to this purpose [1], from the inclusion of electron-phonon interaction [2], to the interaction of the electron with a fixed harmonic oscillator [3], to the introduction of a phenomenological parameter λ, in the very definition of the WF, representing a decoherence length [4].

A new development will be presented related to the study case of an electron beam splitter realized by a potential barrier. A source of noise on the electron kinetic energy in one of the two paths, transmitted or reflected, generates the entanglement of the electron with the environment. At this point, in order to evaluate the diagonal elements of the WF with respect to the environment coordinates, the numerical simulation must interrupt the evaluation of the product of the two lobes of the wavefunction in the two different paths. The stochasticity of the noice source generates a gradual disappearance of the coherent oscillations of the WF.

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Application of the Discrete Wigner Transport Equation to Simulation of Gate-All-Around Silicon Nanowire Transistors: Preliminary Results and Numerical Issues

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Because of easy fabrication and its superior performance over the conventional inversion-mode N^+-P-N^+ junction transistors, the junctionless nanowire transistors (JLNWTs) have been intensively studied, both experimentally and theoretically. To achieve a satisfactory *OFF*-state, the ratio of the gate length (*Lg*) to the silicon channel diameter (2*Rsi*) cannot be too small (≥2). However, there is also a limit to how short *Lg* can be, because of quantum mechanical tunneling through the potential barrier at *OFF*-state. We employ the discrete Wigner transport equation (DWTE) to study such a limit. We simulate gate-all-around silicon JLNWTs of 2*Rsi* = 1.15 nm, oxide thickness *Tox* = 1 nm, highly doped (N_D = 8 x 10^{20} cm^{-3}) contact regions with *Lc* = 3.1 nm on each side, and varying *Lg* = 1.55, 3.1, 6.2, and 9.3 nm, respectively.

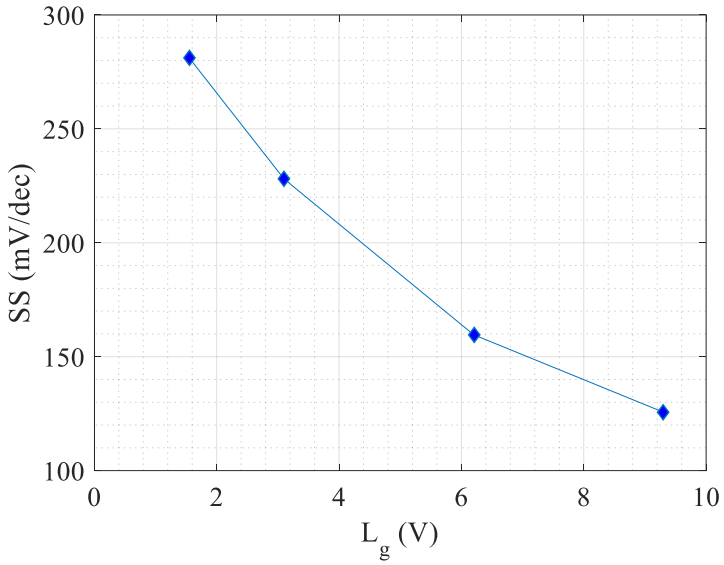

Fig. 1: Variation of the subthreshold slope (SS) depending on the gate length (*Lg*).

Our preliminary simulation results indicate that for a device with *Lg* = 3.1 nm and *Lg*/2*Rsi* = 2.7, the subthreshold slope (SS) is about 228 mV/decade (see Fig. 1), much larger than the ideal value of 60 mV/decade. This calculated value of SS is perhaps over-estimated compared to the actual one because of the limited capability of solving the DWTE beyond the ratio I_{OFF}/I_{ON} ≈ 10^{-3}. We will discuss the origin of this limitation, especially focusing on the problem of accuracy balancing between the discretization of kinetic (diffusion) term and the discretization of potential term in the DWTE [1]. The associated numerical implementation issues will also be discussed.

This research has been supported by the Basic Science Research Program through the National Research Foundation of Korea funded by the Korean government (MSIP) (NRF-2016R1D1A1B03931510).

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Cavity QED of Atoms: Cooling, Trapping and Many-Body Physics

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The elementary system of light-matter interaction is a single atom coupled to a single mode of the electromagnetic radiation field, which is realized in recent cavity QED experiments both in the microwave and optical frequency domain. The so-called strong coupling regime has been achieved, where the coherent interaction between the atom and the field mode due to the electric dipole coupling dominates the uncontrolled dissipation processes. Such a system may have a wealth of applications, e.g. in quantum information processing, where such an atom-field interface can be used as a memory or repeater by converting a flying qubit carried by photons into long-lived hyperfine states of the atom. Capturing an atom inside the tiny volume of an optical resonator is a great experimental challenge not only for technical reasons. The photon scattering in the resonator has a significant mechanical effect on the atomic center-of-mass motion which, in the targeted strong coupling regime, leads to a dynamical coupling between the atomic motion and the field mode amplitude. This effect calls for a substantial extension of the well-established laser cooling and trapping theories. So far, the most transparent and computationally the most powerful approach to describe the dynamics of atomic motion in a strongly coupled field mode is based on the joint Wigner quasi-distribution function representation of the cavity QED system. In this talk we review first the semi-classical description obtained from the Wigner function approach. Then we present various effects, easily obtained from this approach, which shed light into the cooling and trapping of atoms in a cavity. In the second part, we consider many-body effects arising when many cold atoms are trapped in the resonator. The atoms interact indirectly, mediated by the cavity field. A peculiar many-body system is at hand where one can make use of the computational power of the semiclassical theory. We show an experimentally observed non-equilibrium phase transition: the atoms evolve into a periodic crystalline pattern bound by the field Bragg scattered into the cavity off the self-organized crystal (Fig. 1). Finally, we give an outlook on the extension of the semi-classical effects to the quantum domain with Bose-condensed ultracold atoms replacing the cold atoms.

This research has been supported by the National Research, Development and Innovation Office of Hungary (K115624).

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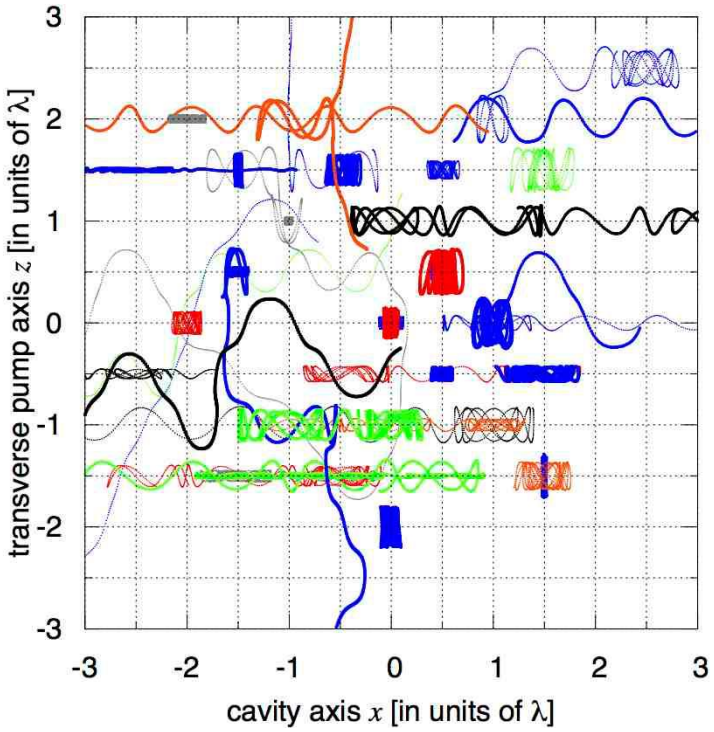

Fig. 1. The initial 5 microseconds of the trajectories of a number of 40 atoms starting from a random homogeneous distribution evolves into a regular pattern occupying antinodes separated by an even number of edges. The atoms along the diagonal lines scatter in phase the laser light incoming from the vertical z direction into the cavity axis direction x. The field building up inside the cavity stabilizes the pattern. The evolution was calculated from the stochastic differential equations generated from a partial differential equation on the joint Wigner distribution function representing the centre-of-mass motion of the atoms and the bossing field mode of the cavity.

Transport Properties of Quasiperiodic Systems

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Quasiperiodic systems and their unique properties attract a lot of attention since the discovery of quasicrystals. Initial interest was mainly focused on their structural properties, but soon afterwards also the transport properties proved to show many interesting features, like the fractal nature of the transmission spectrum [1,2].

The considered model potential profiles are based on two quasiperiodic sequences, Fibonacci and Thue-Morse. Fig. 1 schematically presents those systems: in one-dimensional case both of them shown together with periodic and disordered systems used for comparison, and in two-dimensional case an example of model potential based on the Fibonacci binary sequence.

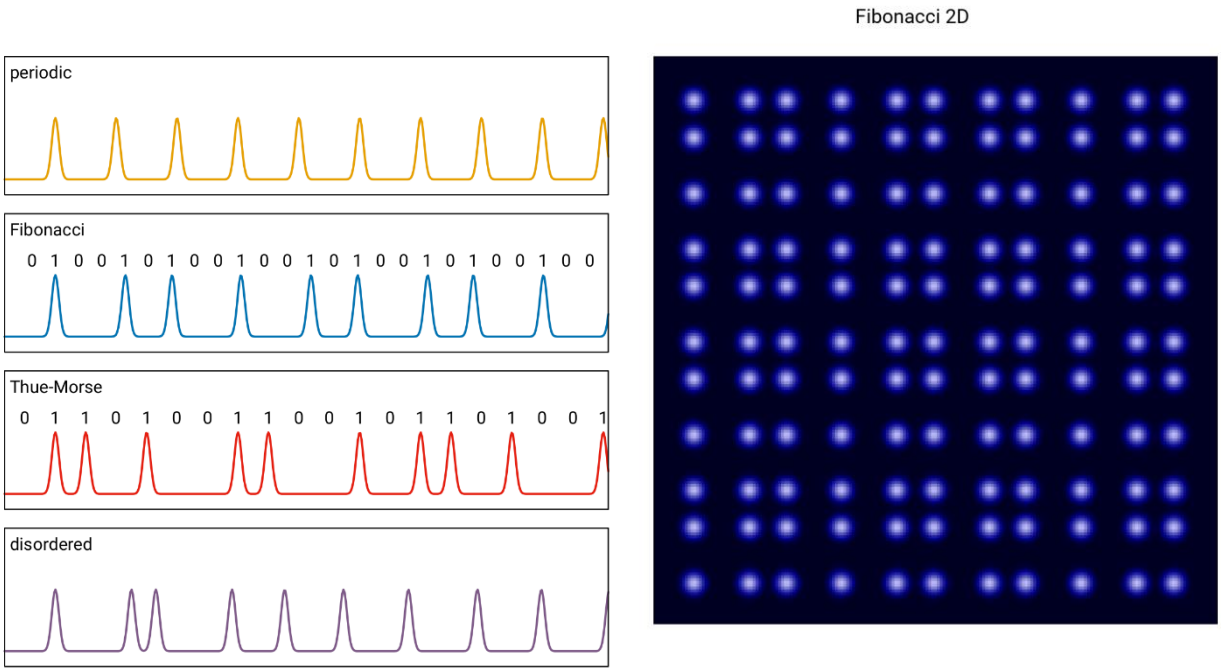

Fig. 1: Left: construction of the model 1D potentials based on the periodic, quasiperiodic and disordered binary sequences. Right: example of the 2D model with scattering centers distributed according to the Fibonacci quasiperiodic sequence.

The methods based on the Wigner function allow us to analyze the dynamics of charge carriers in such systems in the phase space. As a result, we are able to determine the transport properties of quasiperiodic systems, resulting from the quantum phenomena related to the scattering and tunneling processes on potential barriers and/or scattering centers. The time-dependent Wigner functions corresponding to the wave packets traveling in the discussed systems are obtained using methods based on the Wigner equation in the Moyal form [3,4] and with the Monte-Carlo methods using ViennaWD [5]

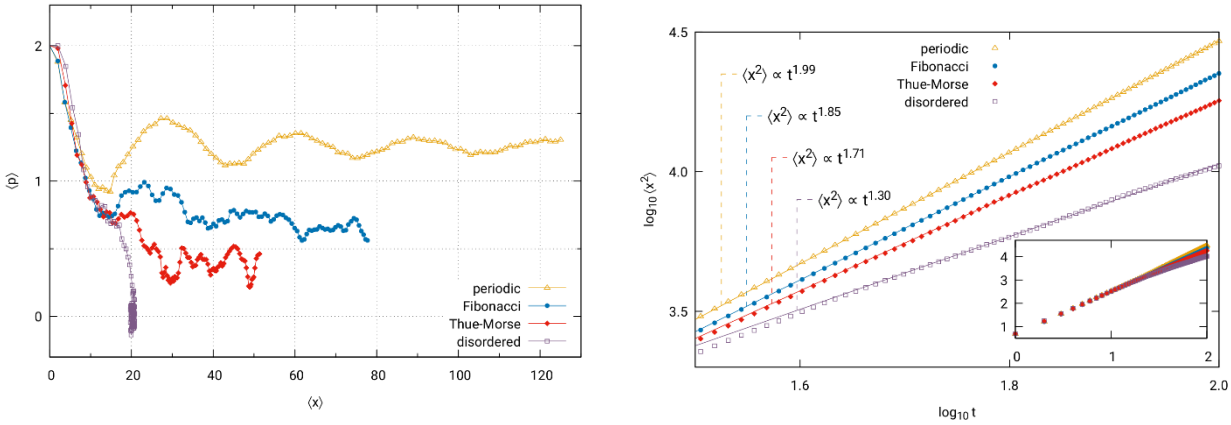

Fig. 2: Left: trajectories in the phase space (in terms of expectation values). Right: diffusion exponents for periodic, quasiperiodic and disordered systems.

The results show that in terms of expectation values of the momentum, position, and their squares, the quasiperiodic systems should be classified somewhere between their periodic and disordered counterparts. Based on the performed calculations, such classification may be based e.g. on the quantitative analysis of the diffusion exponents (Fig. 2).

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The Role of Wigner and Cross-Wigner Functions in a Non-Commutative Phase Space

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In contrast to classical mechanics, which involves a commutative phase space, quantum mechanics uses a configuration space using non-commutative operators. However, one can construct a phase space from pairs of points in configuration space. This phase space inherits a non-commutative *-product, giving a key role to the brackets (f*g-g*f) and (f*g+g*f). This *-product is analogous to the quaternion or Clifford product used for spin structures. The Moyal algebra and the Heisenberg matrix mechanics are particular examples of this general structure. Although the structure is non-local, it gives rise to entities that can be regarded as local operators such as the *local* momentum. These quantities are known generically as 'weak values', which can now actually be measured, giving new insights into quantum phenomena. These weak values are closely related to Wigner and cross-Wigner functions. Our group at UCL are in the process of measuring weak values of spin and momentum using excited helium and argon atoms. My talk will give an overview of this approach.

On the Characteristic Neumann Equation and the Wigner Equation

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For a density matrix $\rho(x_1, x_2)$, the Wigner function $w(r,k)$ is defined as the result of two consecutive transformations:

1. Introduce characteristic coordinates

   $r = (x_1 + x_2)/2$

   $s = x_1 - x_2$

   an define the sigma function

   $\sigma(r,s) = \rho(r + s/2\,, r - s/2).$ (1)

2. Fourier transformation of $\sigma(r,s)$ with respect to s gives $w(r,k)$.

In this work we study properties of the sigma function as defined in (1) and its numerical application to quantum transport problems. Our first goal is a comparison with the finite difference Wigner method [2].

Using coordinates (r,s) the von Neumann-Liouville equation with potential energy V takes on its characteristic form:

$$\frac{\partial \sigma}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial}{\partial r}\frac{\partial}{\partial s}\sigma + U\sigma \quad (2)$$

Here the potential term U is defined as $U(r,s) = V(r + s/2) - V(r - s/2)$. Scattering can be included in a relaxation time approximation using the same model as in the finite difference Wigner method.

Differential equation (2) can be transformed into a two-dimensional integral equation of Volterra type, see [5].

$$\sigma(R,S) = \sigma_0(R,S) + \iint_{00}^{RS} U\,(r,s)drds \quad (3)$$

Here the stationary case is assumed and constants have been absorbed into U. The term $\sigma_0(R,S)$ is a solution to the homogeneous equation and is given by boundary conditions (Goursat or Darboux problem). Existence and uniqueness of the solution to (3) can be proved similarly to the ordinary differential case (expand into a Neumann series and check convergence).

In typical quantum transport problems inflow conditions on left and right boundaries are given. We can impose these boundary conditions through a local Fourier transform. The appropriate choice of boundary conditions for upper and lower boundaries is anti-periodic:

$$\sigma(r, s_{max}) = -\sigma(r, -s_{max})$$

This is consistent with Frensley's discretization as the shifted Fourier transform used in [2] for the Wigner function implies anti-periodic boundary conditions in *s*-space and periodic boundary conditions in *k*-space according to Martucci's classification of discrete Fourier transforms [4].

From (2) we can derive the continuity equation $\frac{\partial n}{\partial t} + \frac{\partial j}{\partial r} = 0$, where local carrier density and current density are given by

$$n(r) = \sigma(r, 0), \qquad j(r) = \frac{-i\hbar}{m}\frac{\partial \sigma}{\partial s}(r, 0).$$

Frensley's discretization in [2] is based on the use of an equispaced *k*-mesh. This is necessary to guarantee conservation of mass which, in the Wigner formulation, is a condition non-local in *k*. In contrast for the sigma equation conservation of mass is a condition local to $s = 0$. Consequently global meshing constraints are less stringent and we are not restricted to the use of an equispaced mesh in *s*. Discontinuities in U resulting from potential steps can be dealt with by using exact matching conditions.

All operators in (2) can be sparsely discretized. In the stationary case (2) can be solved by a shooting method. No big system matrix needs to be stored and the method can easily be parallelized. Sparsity of operators can be exploited which is a major numerical advantage in comparison with the finite difference Wigner method.

There is a large body of knowledge on the numerical solution of hyperbolic equations and on Volterra integral equations [1] [3]. These methods need to be adapted and specialized for use with (2). A further research topic is incorporation of scattering models beyond the relaxation time approximation.

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Wigner Functions for the Canonical Pair Angle and Orbital Angular Momentum

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In view of the impressive successes of Wigner functions on the topologically trivial planar phase space $\mathbb{R}^2$ (and its generalizations to higher dimensions $\mathbb{R}^{2n}$), attempts have been made to generalize the concept to other - topologically non-trivial - phase spaces, in particular, to that of a simple rotator around a fixed axis, its position given by an angle $\theta \in [-\pi,\pi)$ and its angular momentum by a real number p, thus having a phase space corresponding topologically to a cylinder of infinite length, i.e. $S^1 \times \mathbb{R}$.

A main obstacle for the quantum theory of that space for decades has been the treatment of the angle θ which has no satisfactory self-adjoint operator counterpart quantum mechanically. The way around this obstacle is the following [1]: An angle can be characterized by a point on the unit circle which in turn is uniquely determined by the pair $(\cos\theta, \sin\theta)$. The three Poisson brackets of the 3 classical "observables" $\cos\theta$, $\sin\theta$ and p form the Lie algebra of the Euclidean group $E(2)$ of the plane. The unitary representations of this group provide the basis for the quantum mechanics of the system [1]. Its Hilbert space consists of square - integrable functions $\psi(\varphi)$ on the circle with scalar product

$$(\psi_2,\psi_1) = \int_{-\pi}^{\pi} \frac{d\varphi}{2\pi}\, \psi_2^*(\varphi)\, \psi_1(\varphi), \text{ basis: } e_n(\varphi) = e^{in\varphi}, n \in \mathbb{Z}.$$

On this Hilbert space the operators $C = \cos\varphi$ and $S = \sin\varphi$ act as multiplication operators and the angular momentum operator is given by $L = (\hbar/i)\partial_\varphi$ ($\hbar = 1$ in the following). Using this group theoretical structure allows for a consistent construction of the Wigner function $V_\psi(\theta,p)$ associated with a wave function ψ [2,3]:

$$\begin{aligned} V_\psi(\theta,p) &= \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi} d\vartheta\, e^{-ip\vartheta}\psi^*(\theta-\vartheta/2)\,\psi(\theta+\vartheta/2) \\ &= \sum_{m,n\in\mathbb{Z}} c_m^* V_{mn}(\theta,p) c_n,\ \ \psi(\varphi) = \sum_{m\in\mathbb{Z}} c_m e_m(\varphi),\ \ c_m = (e_m,\psi) \\ V_{mn}(\theta,p) &= \frac{1}{2\pi}\, e^{i(n-m)\theta}\ \mathrm{sinc}\ \pi[p-(m+n)/2],\ \ \mathrm{sinc}\ x = \frac{\sin x}{x}. \end{aligned}$$

The "cylindrical" Wigner function $V_\psi(\theta,p)$ has most of the structural properties well-known from the "planar" one $W_\phi(q,p)$. Examples:

The marginal distributions $|\psi(\theta)|^2$ and $|c_m|^2$ are obtained by appropriate integrations of $V_\psi(\theta,p)$ over p and θ, with the sinc function $\mathrm{sinc}\pi(p-m)$ interpolating between the continuous classical values p and the discrete quantum mechanical values $m \in \mathbb{Z}$ of the angular momentum. The transition probability for $\psi_1 \leftrightarrow \psi_2$ is given by

$$|(\psi_2,\psi_1)|^2 = 2\pi \int_{-\infty}^{\infty} dp \int_{-\pi}^{\pi} d\theta\, V_{\psi_2}(\theta,p)\, V_{\psi_1}(\theta,p)$$

and the expectation value of an operator O by

$$\langle O\rangle_\psi = (\psi, O\psi) = 2\pi \int_{-\infty}^{\infty} dp \int_{-\pi}^{\pi} d\theta\, V_\psi(\theta,p)\, \mathrm{tr}[O\cdot V(\theta,p)]$$

Thus, the phase space function ("symbol")

$$\tilde{O}(\theta,p) = 2\pi\, tr[O\cdot\, V(\theta,p)]$$

corresponds to the Hilbert space operator O.

Conversely, given the function $\tilde{O}(\theta,p)$, the operator O is given by

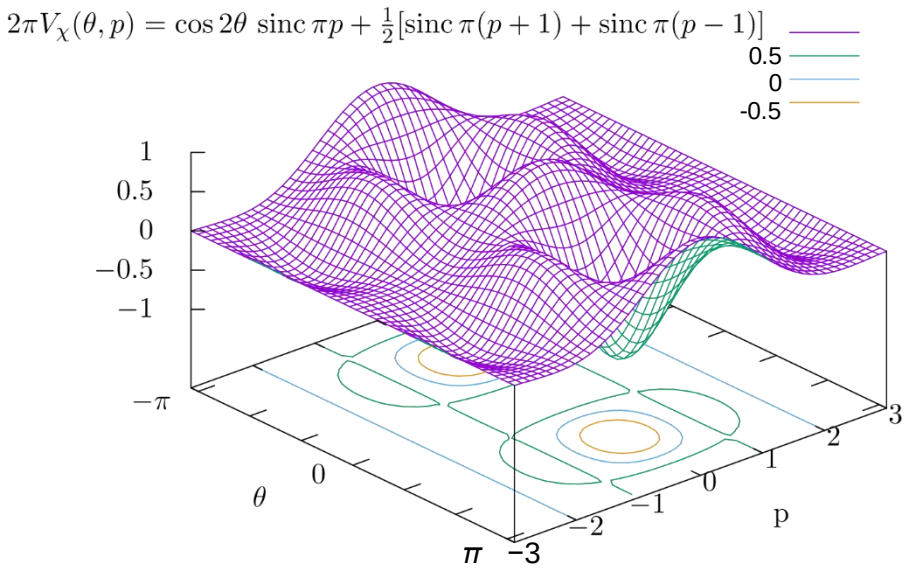
$$O = (O_{mn}) = \int_{-\infty}^{\infty} dp \int_{-\pi}^{\pi} d\theta\, V(\theta,p)\, \widetilde{O}(\theta,p),\ V(\theta,p) = (V_{mn}(\theta,p))\ .$$

Many more relations are discussed in Refs. [2] and [3].

An informative and illustrative example is the Wigner function $V_\chi(\theta,p)$ of the "cat" state $\chi(\varphi) = [\exp(i\varphi) + \exp(-i\varphi)]/\sqrt{2}$:

$$V_\chi(\theta,p) = \frac{1}{2\pi}\{\cos 2\theta\ \mathrm{sinc}\,\pi p + \frac{1}{2}[\mathrm{sinc}\,\pi(p+1) + \mathrm{sinc}\,\pi(p-1)]\}.$$

The θ-dependent term in $V_\chi(\theta,p)$ represents the entanglement of the two superposed basis states $\exp(i\varphi)$ and $\exp(-i\varphi)$ [2].



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Wigner Functions as a Route to Correlation Fluctuations in Problems of Electromagnetic Interference and Noise and Vibration

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Problems of transport of quantum density operators and associated Wigner functions have analogues in classical wave problems that are often of immense practical importance in engineering contexts. Such applications include the propagation of electromagnetic emissions from electronic circuitry, the modelling of wireless/mobile communications in buildings and urban environments, or the prediction of noise and vibration in complex structures such as cars, trains and ships.

In the high-frequency regime, the complexity and scale of these problems typically make direct modelling of the underlying wave problem infeasible, even with the most intensive computational resources. For example, in the context of future 5G communication, it is proposed to exploit frequencies of the order of 60 GHz that have (sub-cm) wavelengths that are extremely small compared to the scale of the environments in which one operates. Even if direct modelling of such problems were feasible, inherent uncertainty in the geometry and other characteristics of the structures involved would make prediction of the detailed response irrelevant. Instead, approximate, course-grained methods such as ray tracing may provide the only practical means of simulating such systems. In this context, efficient numerical propagation of associated phase space densities has been achieved in such complex and large-scale problems using Dynamical Energy Analysis (DEA) and Discrete Flow Mapping (DFM) methods [1,2]. Such complex classical wave systems then provide analogue problems to the quantum-to-classical limit, including environmental uncertainty.

The analogy to quantum transport has received further impetus by the recent emergence of direct measurement of field-field correlation functions as a practical means of characterising electromagnetic emissions from electronic circuits [3-6]. Essentially, the statistically characterised source of such emissions is then modelled by a density operator, in direct analogy to quantum mechanics, and the associated Wigner-function representation has proved effective in modelling its propagation, for example [5-6].

The aim in the work to be presented is to further exploit the connection offered by Wigner-function approaches, between measured correlation functions and phase space densities, to characterise fluctuations in the response of the system. Straightforward ray tracing predicts the averaged response of the system, but not fluctuations due to multipath interference, which can be a dominant feature of the problem and are of tremendous importance in engineering contexts. On the other hand, as previously mentioned, it is typically pointless to predict such fluctuations in detail, as there is usually significant inherent uncertainty in the system structure. We therefore adopt a combined approach, using propagated phase-space densities to predict coarse-grained averaged responses, but adding statistical modelling of fluctuations around this average using Random Matrix Theory (RMT) approaches [7]. The Wigner function representation is essential in achieving this as it provides a direct route from the modelled phase space densities to the correlations and intensities that are of direct interest in applications

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To Know, or not to Know the Quantum State of an Open System, that is the Question in the Realistic Modelling of Quantum Dissipation

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The many-body state for a closed quantum system is computationally inaccessible. Therefore, most approaches for simulating quantum dissipation deal with open systems whose quantum nature is described by a reduced density matrix or a Wigner distribution function. Their equations of motion require a collision term whose exact shape is unknown and requires approximations that, in some cases, can lead to unphysical results [1-3].

The ultimate reason of such unphysical results is that the equation of motion of the Wigner distribution function or the density matrix with the collision terms (interpreted as a dynamical map) can fail to satisfy complete positivity [1]. On the contrary, the condition of complete positivity is trivially satisfied when the density matrix (or its Wigner-Weil transform) can be written, at any time, as a sum over different states $\Psi_j(x,t)$ of the open system, for $j=1,\ldots,W$, as:

$$\rho(x,x') = \sum_j p_j \Psi_j^*(x',t) \Psi_j(x,t) \quad (1)$$

where p_j is the probability of each of these states. Eq. (1) directly implies a positive density operator and a completely positive map [1]. Unfortunately, the states $\Psi_j(x,t)$ of an open system are inaccessible within the "orthodox" formulation (the reduced density matrix in Eq. (1) is defined as an improper mixture [4]), unless the environment is continuously monitored as done in Stochastic Schrodinger equation techniques [5].

In this conference, I will show how the Bohmian formulation of an open system [6,7], allows an alternative and *natural* definition of the (conditional) wave functions of an open system, $\Psi_j(x,t)$, where the subindex j accounts for different experiments. With the knowledge of the state of the open system, $\Psi_j(x,t)$, it is a straightforward procedure to develop a quantum approach for dissipation that, by construction, satisfies Eq. (1) and therefore provides a complete positive map for either Markovian or non-Markovian dynamics. In this conference, I will also explain how such approach can be implemented to study dissipation and decoherence in tunnelling devices with either linear (Dirac equation) or parabolic (Schrödinger equation) band dispersions [8,9]. The details and capabilities of this approach are indicated in Figs. 1 and 2.

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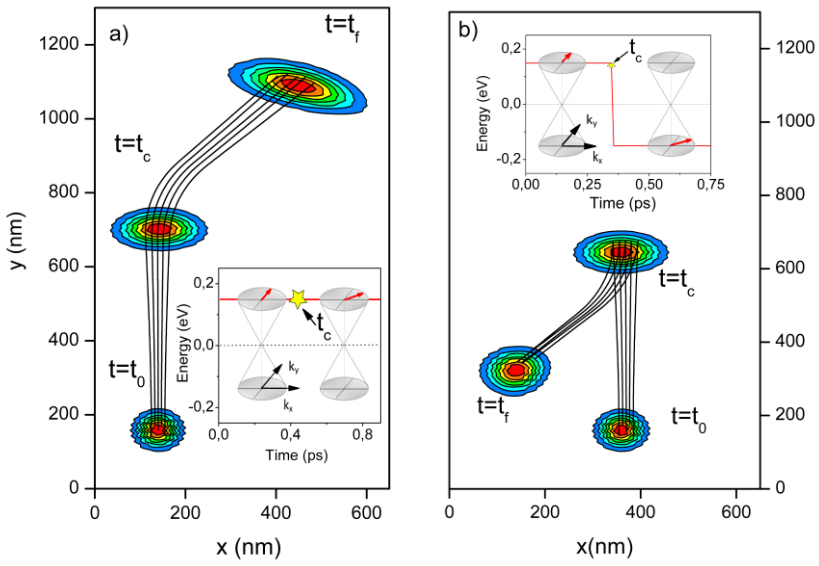

Figure 1: a) Time evolution of the modulus squared of the conditional wave function of an electron in the conduction band of a graphene sheet with initially wave vector $(k_{xo},k_{yo})=(0,2.27e^{-8})$ m^{-1} suffering an elastic collision (at t_c) with a phonon that lead to a final wave vector $(k_{xf},k_{yf})=(1.6e^{8}, 1.6e^{8})$ m^{-1}. The associated Bohmian trajectories are also plotted. Inset: Energy conservation of the elastic collision. **b)** Same wave vector change as in a) but with an inelastic collision that moves the electron to energies in the valence band (with opposite velocity and momentum) as seen in the energy inset.

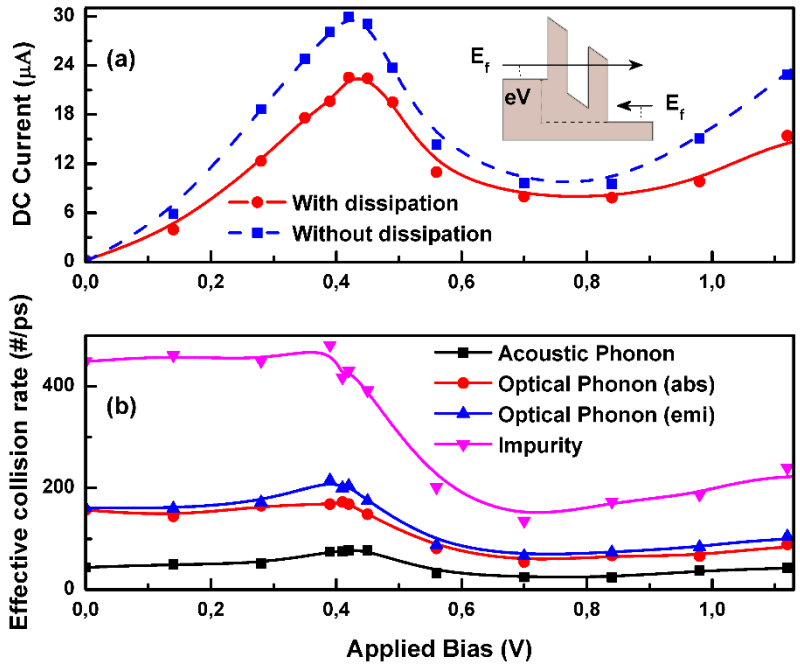

Figure 2: a) Current-voltage characteristic for a resonant tunnelling diode with (solid red curve) and without (blue dashed curve) dissipation due to (acoustic and optical) phonons and impurities. The optical phonons leads to an inelastic electron energy change of ±0.036 eV. The simulation time for each bias point is 5 ps. The Fermi energy is E_f=0.15 eV and the electron effective mass $m^*=0.067m_0$ with m_0 the free electron mass. The barrier height and width are 0.5 eV and 1.6 nm, respectively, and the well width is 2.4 nm. **b)** Number of collisions as a function of bias. At resonance, the number of collisions is three times greater than out of resonance.

Non-Classical Properties of Electronics States. Influence of the Scattering Mechanisms

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In the phase-space representation of quantum mechanics the quantum state of the system cannot be represented by the Dirac measure localized at a point in the space because of Heisenberg's uncertainty principle. In this framework, the quantum state of the system can be represented by the Wigner quasi-probability distribution function or simply the Wigner function, and dynamical variables form a non-commutative algebra on the phase space [1]. This formulation of quantum mechanics is frequently used as an alternative to the description of the electron's dynamics in the condensed matter nanosystems where the analysis based on the ordinary Boltzmann's picture of transport phenomena is rather inadequate. One of the reasons for this uncomfortable situation is the inherence of the quantum interference phenomena which introduce the effect of the phase memory for propagating electrons through the nanosystem over a distance which is called the coherence length.

The quantum interference between spatially correlated pieces of electronic states in the phase space is related to the negative part of the Wigner function [2]. From the mathematical point of view the negative values of the Wigner function can be regarded as a consequence of the Weyl transform of the density matrix, which transfers the off-diagonal elements of the density matrix in the position representation to the momentum variables [3]. This procedure suggests the existence of the mutually dependent correlations between the momentum and position states of conduction electrons.

In this report, the problem of the position-momentum correlations in the phase space is discussed. We present a scheme for determination of these correlations using the methods based on the Wigner function. For this purpose the appropriate class of correlation functions is defined and some of them are numerically calculated for the canonical system of nanoelectronics, which is a resonance tunneling diode [4]. The preliminary results are presented in Fig. 1.

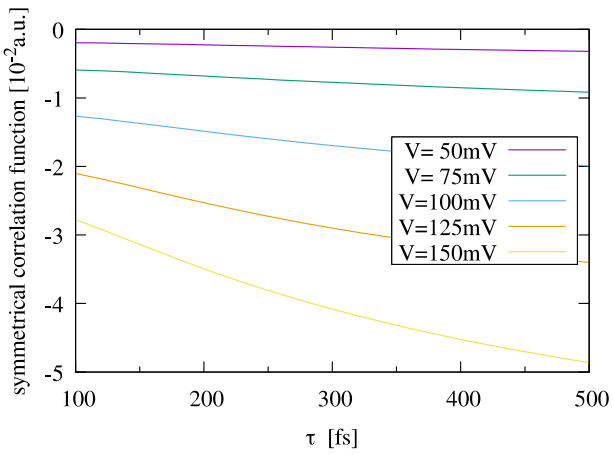

Fig. 1: Influence of the relaxation time on the symmetrical correlation function of the first order at selected points of the current-voltage characteristics.

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Apart from this, we also investigate the influence of the scattering mechanisms on non-classical properties of electronic states. It allows us to analyze the evolution of quantumness of the states driven by the bias voltage along the current-voltage characteristics.

All the obtained results are discussed based on steady-state solution of the kinetic equation with the scattering integral in the form of the relaxation time approximation for the Wigner function. Additionally, a short discussion of the time evolution of the non-classical properties of the electronic state in the quasi-ballistic regime is included. For this purpose, the Wigner equation in the Moyal form is solved [5, 6], and the dynamical aspects of electronic states which stem from its quantumness are analyzed.

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A Probabilistic Model for the Wigner Transport Equation

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The term Wigner Monte Carlo method is used for the “particle based Monte Carlo approach to the Wigner–Boltzmann transport equation”. During these years, several variants of the method related to particle weights (signed, integer valued, continuous) have been introduced [1].
This paper is concerned with the construction of a probabilistic model for the Wigner equation. The model is based on a particle system with the time evolution of a piecewise deterministic Markov process. Each particle is characterized by a real-valued weight, a position x and a wave-vector k. The particle position changes continuously, according to the velocity determined by the wave-vector. New particles are created randomly and added to the system. The main result is that appropriate functionals of the process satisfy a weak form of the Wigner equation. Moreover the stochastic model contains several new algorithms as well as some of the algorithm previously considered in the literature. The approximation error and the efficiency of the algorithms are analyzed and performed on a benchmark test case, where certain advantages of the new class of algorithms are demonstrated.

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Self-Energy Approach for Solving the Wigner-Transport Equation

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An efficient numerical solution of the Wigner-transport equation based on the Wigner-Weyl transformation is desirable. Unfortunately, conventional approaches suffer from different drawbacks. On the one hand the drift operator represents a function, which oscillates strongly due to the spatial frequency leading to high approximation errors as the Fourier integrals within the Wigner-transport equation are not converging with respect to the Hartree-Fock potential [1]. On the other hand so-called upwind difference methods are used for the numerical approximation, which overestimate diffusion effects [2]. Therefore, coherent effects cannot be described adequately and inherent errors are a consequence. Furthermore, local boundary conditions are assumed, which neglect the non-local behavior of quantum mechanics [3]. Open boundary conditions are needed. The numerical results deviate from the results obtained by coherent models when scattering is neglected [4].

An approach is presented, which circumvents the above mentioned issues. The von-Neumann equation in center-mass coordinates r and r' is discretized by means of a finite volume technique. The discretization pattern is based on ideas coming from propagator expansions for electromagnetic field calculations. The computational domain is divided into cells in r-direction, for which the discretized von-Neumann equation is formulated consisting of a discretized diffusion and drift operator. For each cell, the solution in r'-direction is expanded dependent on the eigensolutions of the discretized diffusion operator, which represent inflow and outflow waves. Self-energies accounting for open boundary conditions in r'-direction can be incorporated. The matrices for each cell can be combined to form a system matrix for the whole computational domain. The resulting matrix equation describes the numerical problem dependent on the r-direction and dependent on the boundary conditions in r-direction. Due to the introduction of inflow and outflow waves, additional self-energies in r-direction can be defined. The basis of the discretized diffusion matrix can be chosen in a way that the eigensolutions correspond to the Weyl transform, so that the characteristics of the conventional Wigner-transport equation can be preserved.

The von-Neumann equation is self-consistently solved along with the Poisson equation for a resonant tunneling diode (Fig. 1) at an applied voltage of 0.11V. The density matrices are determined for the proposed approach and the conventional approach solving the Wigner-transport equation based on an upwind difference scheme. These methods are compared with each other, whereby for both methods the real (Fig. 2) as well as the imaginary part (Fig. 3) of the density matrices are depicted as a function of the center-mass coordinates. The difference between both approaches can be observed from both figures. The results achieved with the proposed approach correspond very precisely to the solution obtained by the Schrödinger equation, so the results of the latter approach are not shown. The current density cannot be correctly determined by the conventional Wigner-Weyl approach. This statement can be concluded from the imaginary part of the density matrix (Fig. 3b) due to the different derivatives in r '-direction when considering the location r' = 0.

Finally, an approach is presented, which avoids the above mentioned major problems of conventional numerical methods for solving the Wigner-transport equation and exploits the advantages of the self-energy-concept, which is quiet common when using non-equilibrium Green's function approaches. The approach offers the possibility to allow a computationally efficient design of nanoelectronic devices.

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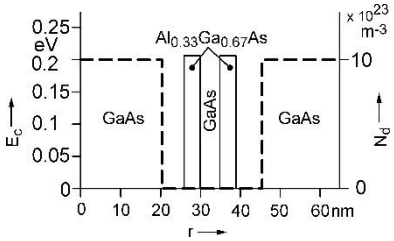

Fig. 1: Energy band E_C for the RTD and doping concentration N_d.

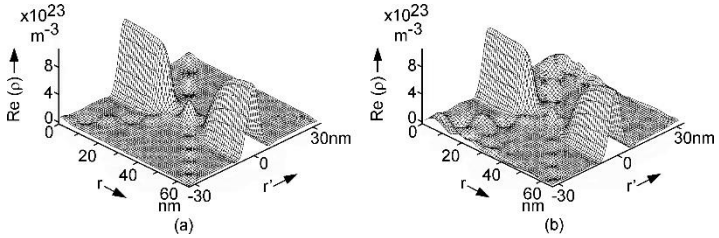

Fig. 2: Real parts of the density matrix for the proposed approach (a) and the Wigner-transport equation (b).

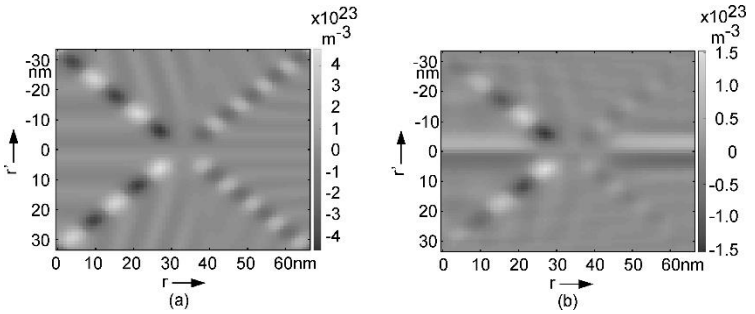

Fig 3: Imaginary parts for the proposed approach (a) and the Wigner-transport equation (b).

Wigner Analysis of Surface Roughness in Quantum Wires

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Surface roughness (SR) is the low field electron mobility limiting mechanism in confined structures. Classical (Monte Carlo) transport models describe the effect of the electron interaction with the surface imperfections in terms of the Fermi Golden Rule, characterized by the stationary (long time) limit of the interaction process giving rise to the energy conserving delta function, and a statistical averaging which provides a position-independent scattering probability. An alternative approach, which allows a deep insight in the processes governing time-dependent, quantum electron dynamics in presence of SR, is based on the signed particle model [1], which provides an equivalent autonomous formulation of the Wigner theory [2]. The model retains many classical notions like phase space and point-like particles which drift and scatter like Boltzmann particles. The quantum information is carried by positive or negative sign [3] used to evaluate the physical averages. Particles generate - according to rules defined by the Wigner potential - couples of novel signed particles. Their inertial motion is not affected by the potential, in particular the electric field does not cause any acceleration. The signed particle model is utilized via *ViennaWD* [4] for a comparative study of quantum evolution in ideal and rough-surface wires. Identical Wigner states $f_w = Nexp\{-(r-r_o)^2/2\sigma^2\}\exp\{-(k-k_0)^2 2\sigma^2\}$, injected with a period of $5\ fs$, are centered in the source contact of the wire. The governing physical process is tunneling, there are no artificial walls which stop or reflect the particles: On the contrary, particles are removed after reaching the domain boundaries. Fig.1 shows that the electron density is not evenly distributed even in the ideal case. The initial penetration into the walls is followed by a reflection and further shrinking of the channel towards the drain ($y = y_{max}$). The SR pattern in Fig.2 (left) is generated by the function $L_0\exp\{-\Delta x/c_l\}$ [5] with the mean offset L_0 and the correlation length c_l. The electron evolution is retarded by the roughness so that the density at the drain becomes stationary after $200\ fs$. It is well seen how the density is reshaped by the variations of the potential. Fig.3 presents the difference between the ideal and rough marginal distributions $fi_w(k_y,*) - fr_w(k_y,*)$ where $*$ denotes the integration over x, y and a sum over (the discrete values of) k_x. The fact that $fi_w(k_y,*)$ remains unaffected during the evolution (due to the y-independence of the potential) provides a reference for the analysis: The existence of negative wave vector values prompts for quantum reflection, where $fi_w(k_y,*)$ values dominate. The major conclusions are that far from equilibrium the conditions along the wire become inhomogeneous and that quantum reflections are caused by the SR. Another effect is the reduction of the speed in the transport direction as confinement keeps the density away from the interface thus reducing the SR effect.

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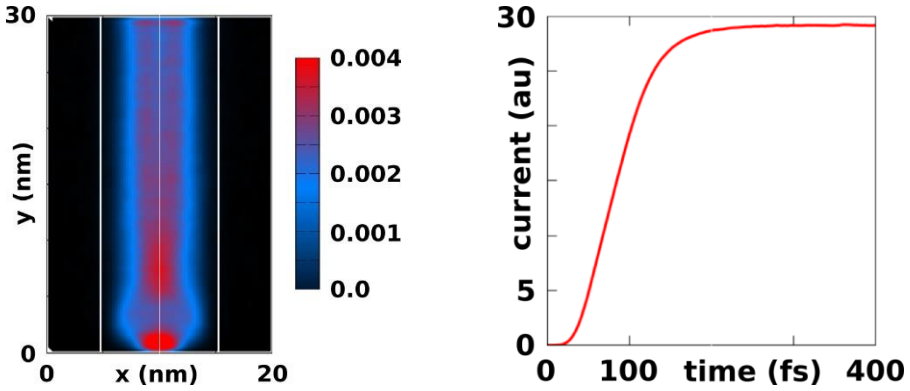

Fig. 1: The ideal wire walls are formed by $5\ nm$ wide $0.8\ eV$ potential strips which smoothly drops to 0 in the next $2\ nm$ towards $x = 10\ nm$. The injected states use $r_0 = (10, -4\sigma)\ nm$ and $\sigma_{x,y}$ of $2\ nm$ corresponds to the equilibrium at $300\ K$. A stationary picture of the density (in arbitrary unit) is reached after $175\ fs$ injection, when the current enters the $3\ \%$ limits around its mean value.

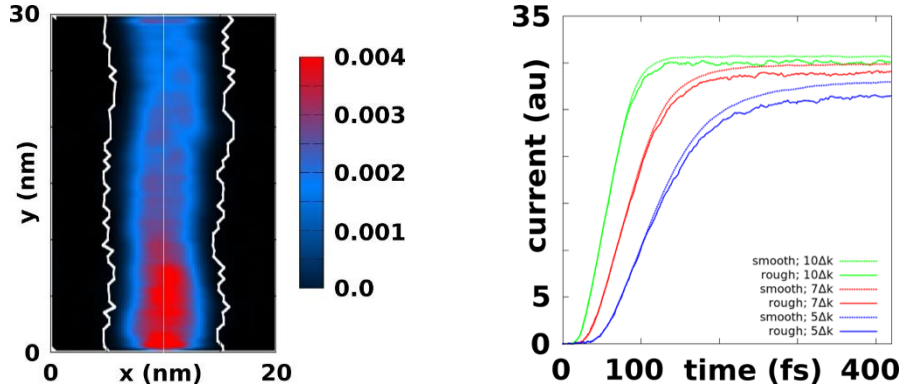

Fig. 2: The SR density (in arbitrary unit) pattern with $5\ nm$ correlation length and $0.5\ nm$ mean offset causes a reduction of the current, given on the right picture for three different values of $k_{0,y}$; Δk corresponds to $1\ meV$.

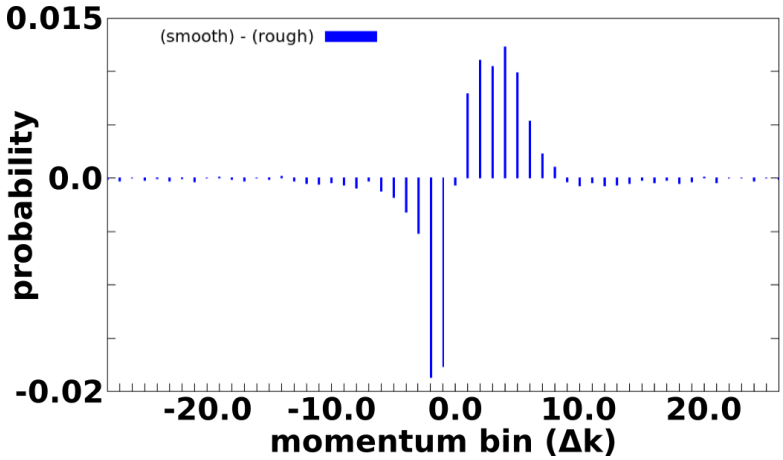

Fig. 3: The difference between the ideal and rough marginal ky-distributions shows a reduction of the speed in the transport direction and a reflection caused by the SR varying potential.

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Numerical Aspects of the Deterministic Solution of the Wigner Equation

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Quantum mechanical effects in the carrier transport processes have to be accounted for during the development of modern and future electronic devices. A convenient formulation is provided by the Wigner formalism [1,2]. Especially for problems where phase-space quantities vary over several orders of magnitudes deterministic solution methods [3] are favored over stochastic approaches. The problematic discretization of the diffusion term triggered the development of an approach which utilizes an integral formulation of the Wigner equation [4]. In general, the developed method describes the evolution in time as the superposition of the time evolution of several fundamental wave packages.
Major considerations are necessary to overcome the memory and time demands typical for the modeling of any quantum transport method [5].
Through an examination of the resulting equations it was possible to dramatically reduce the complexity of the equation system and a final reduced set of equations resulted. However, due to the computational costs of the solving mechanism a parallelization of the procedure is essential and through this approach made possible. Depending on the problem type several solution approaches are feasible which affect the discretization and offer further possibilities for optimization.
Several aspects of the numerical consequences of this approach will be discussed.
For simple problems with a time invariant setup each fundamental evolution can be computed independently, collecting all fundamental solutions to the entire one. Parallelization among the partial processes is made possible.
If a dependence of the partial evolutions is caused, for instance by scattering, the partial processes may be calculated in parallel but the synchronization of and the communication between the processes is required.
If the applied potential stays constant, the partial updates stay constant as well. In this case the partial updates may be calculated only once and applied to the distributions of the previous time-step. However, In this case a communication of the actual solution among the processes has to be triggered.
Depending on the chosen method different computational issues may arise. To achieve the results in reasonable time attention has to be kept on the (at least) second order dependence of spatial and k-space resolution on calculation times. Due to the high dynamic of the solution it may be also necessary to apply a dense time-spacing. Accordingly, in areas of low velocities, due to numerical reasons, the discrete trajectories may stop evolving.
This aspect may not be harmful using stochastic methods. These areas move their discrete position with low probability. In the deterministic version this instance is accounted for by adapting the velocities by their cumulative error in the trajectory in time.
However, for the one-step method, the trajectory update is only calculated once. In this case an interpolation of the solution achieves a result. Attention has to be paid to the fact that information is lost and edges may broaden during this interpolation. In Fig. 1 sample simulations by applying the developed method are shown for a wave packet passing through a 0.1eV potential barrier and through two 0.05V potential barriers.

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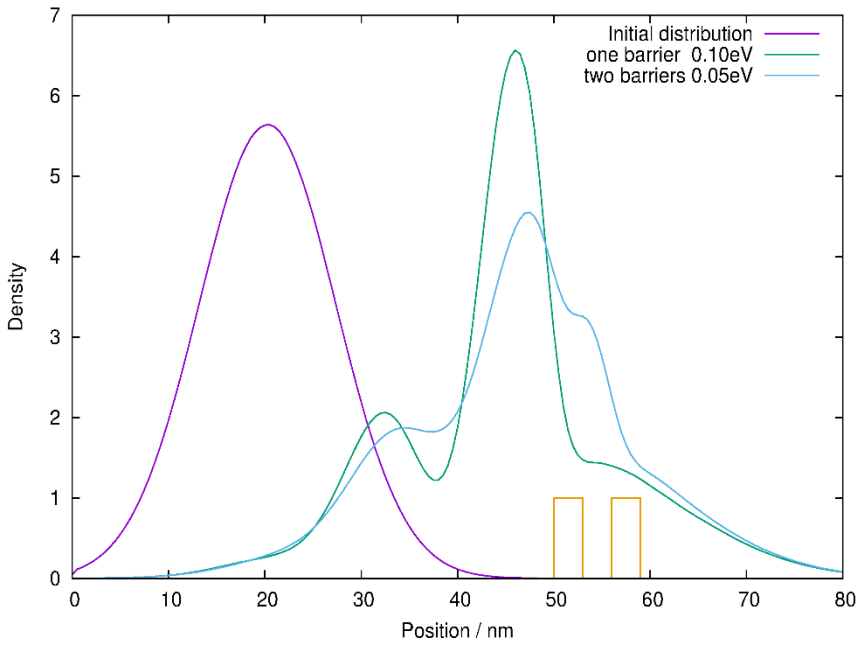

Fig. 1: Two simulations of a wave packet passing through a 0.1eV potential barrier and two 0.05eV barriers are shown at time=0s and after 100fs. In this case the one-step algorithm, in combination with interpolation, achieves best results.

Accurate Deterministic Wigner Functions for Typical Quantum Systems

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The Due to the higher dimensionality and the oscillating structure of the Wigner function, highly accurate deterministic numerical simulations have been almost exclusively confined in 2D phase space and few results are reported in a higher dimensional phase space, even for a 4D system. Recently, we proposed an advective-spectral-mixed method for the 4D problem with a bounded and fast decay potential [Ref: SIAM J. Sci. Comput. 38 (2016) B491-B520]. In virtue of the operator splitting technique, we now extend the method into the problems with non-decay potentials and obtain accurate Wigner functions in dealing with the the double-well potential as well as in simulating directly the double-slit experiment and others.

Efficiency and Numerical Challenges on the Resampling Techniques in Stochastic Wigner Simulations

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Towards to an efficient Wigner branching random walk (i.e., signed particle Wigner Monte Carlo) simulation in high dimensional (>=6D) phase space, the resampling procedure (particle cancelation) plays a key role, which is usually made up of two parts: an appropriate particle reduction method to control the particle number and an accurate sampling strategy from the resulting density estimation. By exploiting the idea of non-parameter density estimation method in statistics, we would like to formulate the resampling as a histogram approximation, as well as a piecewise constant reconstruction of the Wigner function. Theoretical analysis validates the consistency of the proposed method and numerical results demonstrate the reliability when the dimension of phase space is moderately large (for instance, 4D). However, we also point out the potential weakness and challenges of such resampling strategy in higher dimensional problems.

A Wigner Equation with Decoherence

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The quantum dynamical decoherence of a “heavy” particle interacting with a single “light” particle, is studied in detail in Ref. [1]. Starting from this two-body problem, we consider a quantum particle that interacts with a gas of light particles, and we derive the effective evolution of the reduced Wigner function. Our model includes in a natural way a decoherence mechanism, which turns out to be the generalization of analogous mechanisms already considered by Joos and Zeh [2], and even proposed by Wigner himself [3]. However, our extended formalism allows to introduce, at least on a phenomenological ground, a “saturation” of the decoherence process in the long run.

In our contribution we briefly report on the derivation of the model as well as on some of its mathematical and physical properties, including energy and momentum dissipation rates, also with the help of simple numerical examples. Moreover, we discuss the relationships of our approach with the above-mentioned references [2] and [3], and with approaches based on Wigner functions with finite coherence length [4]. Finally, we indicate some possible extensions and directions for future investigation.

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Wigner-Signed Particles Study of Double Dopant Quantum Effects

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We investigate the quantum effects induced by two dopants positioned on the electron path in a structure which resembles a two-dimensional quantum wire. We use the signed particle model for analysis, which presents an alternative heuristic formulation of the Wigner transport picture [1]. The major attributes of the model are that point-like particles with classical features, such as drift over Newtonian (field-less) trajectories, carry the quantum information by their positive or negative sign which contributes to the physical averages $< A >$, which, apart from the sign, can then be calculated as in the classical case. The Wigner potential determines a spatial probability map, according to which any particle generates two novel counterparts with a positive and negative sign, while the attributes of the initial particle remains unaffected [2]. Contrary to Boltzmann particles, which resemble electrons, signed particles bear a mere numerical character. In particular, the electron density in a given phase space unit cell is approximated by the difference of positive and negative particles. With the double dopant experiment we analyze the effect on the electron density by continuously injecting identical, minimum uncertainty Wigner states $f_w = Nexp\{-(r-r_o)^2/2\sigma^2\}\exp\{-(k-k_0)^2 2\sigma^2\}$ [3], aiming to maintain coherent conditions. Since any injected state may be interpreted as a classical distribution, we can conveniently use the Boltzmann picture as a reference frame: Classical particles move on un-accelerated Newtonian trajectories until closing in on the dopants, where they begin to feel the electric force (cf. green area in Fig. 1). After leaving the region the free movement continues until leaving the domain. The particle transport is mainly along the y-direction (from bottom to top), the correlation between the two symmetric left and right subdomains (i.e. $0 \leq x \leq 10nm$ and $10nm \leq x \leq 20nm$) happens merely between the dopants and the drain (i.e. $y = y_{max}$). We use quantum simulations, powered by *ViennaWD* [4], to provide a density distribution as shown in Fig. 2. In particular, r_0 is centered in the source contact ($x = 10nm$) of the wire and $\sigma_{x,y} = 2nm$, corresponding to the equilibrium distribution around k_0 with the effective mass $m^* = 0.19$ at $T = 300\,K$, with a total simulation time of $400\,fs$ and an injection period of $8\,fs$; steady state is reached after about $200\,fs$. To study processes giving rise to coherence, we perturb the correlation between the two subdomains by introducing an artificial *kill zone* along the vertical symmetry line within the area $9.5nm \leq x \leq 10.5nm$ and $22nm \leq y \leq 25nm$, where negative particles are eliminated. Such a perturbation does not affect the classical picture since, as discussed, there is no correlation between the subdomains separated by the kill zone, there are no negative particles. Furthermore, if the action of the Wigner potential, which ensures the coherence, is weak, the effect of such a kill zone can only increase the electron density. Fig. 3 shows the effect of the kill zone on the density distribution (compare to Fig. 2). For a more detailed analysis, Fig. 4 shows a comparison of the density along $y = 29\,nm$: For the kill zone case (red dashed line) the results show the opposite effect as described above - a reduction of the density. This demonstrates the active role of the Wigner potential in the domain around the kill zone. The main conclusion is, that, in contrast to the classical case, there exists an active particle exchange (i.e. correlation) in the horizontal x-direction, which is of crucial importance for the system to maintain coherence.

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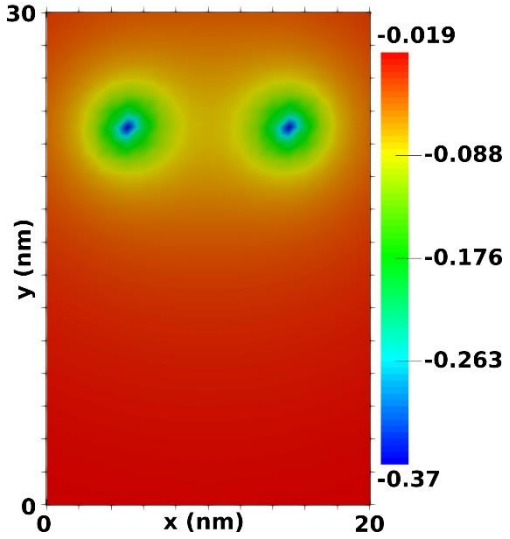

Fig. 1: Potential distribution in eV. The green region outlines the potentials of the two dopants. The setup is such that we can ignore a joint action of the corresponding forces.

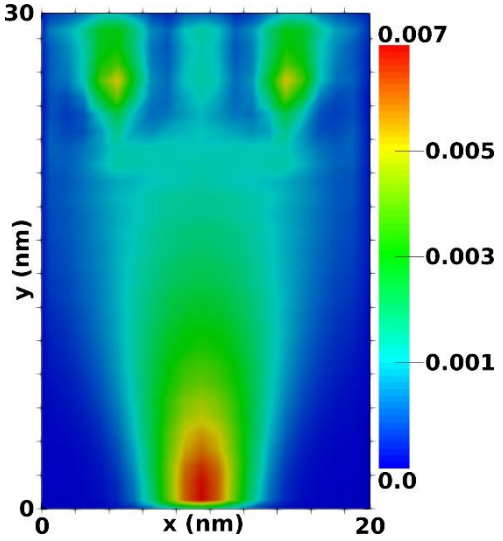

Fig. 2: After $200\ fs$ quantum evolution the density (arbitrary unit) approaches a stationary distribution. No artificial borders are introduced; particles leaving the simulation domain in any direction are eliminated.

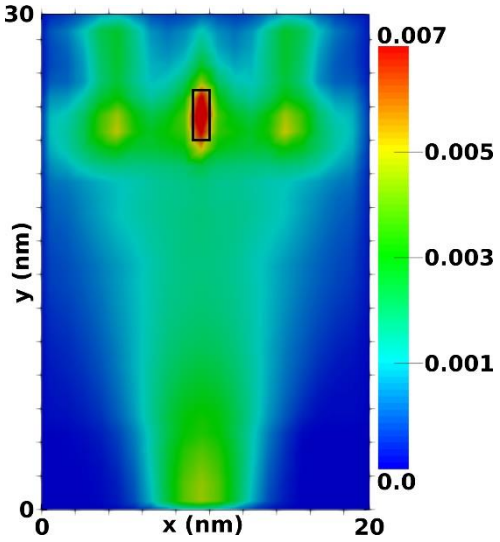

Fig. 3: Kill zone density distribution (arbitrary unit) after $200\ fs$. The black rectangle indicates the kill zone.

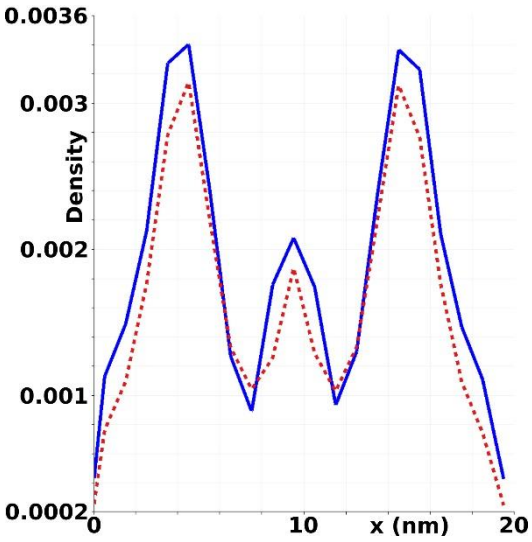

Fig. 4: Comparison of density distribution (arbitrary unit) via a screen at $y = 29\ nm$ after $200\ fs$.

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