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Device modeling in the Wigner picture

Computational aspects

M. Nedjalkov · H. Kosina · P. Schwaha

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Abstract Basic computational aspects of the Wigner function approach for modeling and simulation of electronic transport are discussed, beginning with the coherent problem, followed by the dissipative problem including scattering events, which has been recently restated in terms of a scattering-induced Wigner function correction. These alternative formulations of the computational task are discussed along with a method for separation of the Wigner potential into classical (force) and quantum components.

Keywords Wigner function · Boltzmann scattering · Carrier transport models

1 Introduction

The Wigner picture provides a phase space formulation of quantum theory, where states and observables are represented by functions of the real space and momentum coordinates. The Weyl transform attributes to any given operator of the wave mechanics a phase space counterpart which is a c-number. The Wigner function can be viewed as both, a phase space counterpart of the density matrix and a quantum counterpart of the classical distribution function. Basic notions of the classical statistical mechanics are retained in this picture. In particular the usual quantities of interest in operator quantum mechanics, i.e. mean values and probabilities associated to given physical observables, are evaluated in phase space by rules resembling the formulae of the classical statistics. It is for these reasons that the Wigner function is often apprehended as a quasi-distribution function. The basic difference with the Boltzmann counterpart is the appearance of negative values which characterize correlations and outline quantum from classical transport.

The standard phase space formulation of quantum mechanics has been established historically on top of the operator mechanics [1–3]. The inverse approach, explored later [4, 5] provides an independent formulation of the Wigner theory in the phase space. Conditions are derived, which specify the admissible quantum phase space functions in terms of pure and mixed states, and the rest of non-quantum states. A one to one correspondence is established between the space of all real pure state functions of the phase space and the Hilbert space of the physical states. Furthermore the Weyl transform defines the correspondence between the Hermitian operators of the observables and phase space functions with certain properties. This autonomous formulation of the Wigner theory recovers the operator mechanics, which completes the proof of the logical equivalence between the two approaches [5].

The Wigner function approach has been applied for more than 2 decades to modeling and simulation of transport of charge carriers in electronic structures. Beginning with the coherent problem successfully solved for both stationary and transient conditions, the approach has been generalized to account for scattering events. Relevant for device modeling applications is the stationary problem imposed by stationary boundary conditions. Recently it has been reformulated as an initial condition problem with the help of the scattering-induced Wigner function correction. These al-

M. Nedjalkov (✉) · H. Kosina · P. Schwaha
Institute of Microelectronics, TU-Vienna, Gusshausstrasse 27-29, E360, 1040 Vienna, Austria
e-mail: mixi@iue.tuwien.ac.at

H. Kosina
e-mail: kosina@iue.tuwien.ac.at

P. Schwaha
e-mail: schwaha@iue.tuwien.ac.at

ternative formulations are discussed along with a method for separation of the Wigner potential into classical (force) and quantum components. The method overcomes the divergence of the standard definition due to an applied voltage and ensures a smooth Fourier transform of the quantum component.

2 Formulation of the problem

The standard way of introduction of the main entity of the formalism—the Wigner function—relies on the density operator $\hat{\rho}$ and the corresponding density matrix, which for a single-dimensional (1D) task with a space coordinate x is $\rho(x, x') = \langle x'|\hat{\rho}|x\rangle$.

2.1 Coherent Wigner equation

The Wigner function f_w is defined in the 1D phase space x, p by the Weyl transform of the density matrix ρ. Usually the momentum variable is replaced by the wave number $k = p/\hbar$, giving rise to the following definition:

$$f_w(x,k,t) = \frac{1}{2\pi}\int dx'\,\rho(x+x'/2, x-x'/2, t)e^{-ix'k}. \quad (1)$$

The transform, as applied to the von-Neumann equation for the evolution of the density operator $i\hbar\frac{\partial\hat{\rho}}{\partial t} = [H,\hat{\rho}]_-$ introduces the Wigner equation and the Wigner potential V_w:

$$\frac{\partial f_w(x,k,t)}{\partial t} + \frac{\hbar k}{m}\cdot\nabla_x f_w(x,k,t) = \int dk'\,V_w(x,k-k')f_w(x,k',t), \quad (2)$$

$$V_w(x,k) = \frac{1}{i\hbar(2\pi)}\int dx' e^{-ix'k}(V(x+x'/2) - V(x-x'/2)). \quad (3)$$

The computational approach first requires to evaluate V_w and then to solve (2). Equation (3) usually invokes the theory of generalized functions and needs a numerical evaluation. We postpone the discussion of the theoretical aspects of (3) for the next section. The numerical evaluation is performed by restricting the x' integration to a finite interval L_{coh} called coherence length.

The initial condition problem can be illustrated by the example of a wave packet evolving towards a potential obstacle [6, 7]. The evolving wave packet, a solution of (2), nicely demonstrates the process of tunneling. Already such reversible evolution of a pure state needs a precaution: the equation allows unphysical solutions which must be filtered out. For example in the case of a quadratic Hamiltonian (e.g. a harmonic oscillator) equation (2) reduces to the collisionless Boltzmann equation: solutions violating the uncertainty relation would be possible. The filtering is ensured by the initial condition which must be an admissible quantum-mechanical state. Necessary and sufficient condition for a pure state has been derived in [4], which in conjunction with (2) makes the computational task equivalent to solving the Schrödinger equation. It can be shown that an initial pure state evolved by (2) remains a pure state [4]. This is, however, not true under general physical conditions, if the evolution is provided by the classical counterpart of (2), obtained if the Wigner potential is approximated by the classical force.

Modeling an operating device requires a specification of boundary conditions, describing the coupling with the environment, i.e. the attached leads. Physical boundary conditions are related to injection/absorption of particles to and from the device, which becomes an open system. They provide a necessary condition for irreversibility of the solution of (2): otherwise no stationary states and thus current-voltage characteristics are possible [8]. Here the lack of equivalence with the Schrödinger equation is revealed by another issue: equation (2) augmented with boundary conditions can not describe bound states. Indeed if the system Hamiltonian and a component of the density operator commute, this component dissapears in the von Neumann equation. A way to describe bound states is proposed in [9], where an adjoint Wigner equation is derived and regarded in conjunction with (2) to fully reconstruct the Schrödinger eigenvalue problem. Such states are independent of the changes at a given boundary, as their energy spectrum is below the potential bottom at the boundary.

Another way to include bound states is to sacrifice the ballistic picture and take into account dissipation mechanisms which allow scattering between the different types of states. In this way bound or quasi-bound states may be charged properly by the boundary conditions. It has been recognized that dissipative processes are a necessary part of device physics: if the interplay between coherent and decoherence processes is neglected, the modeled system may show unphysical behavior [10].

2.2 Wigner-Boltzmann equation

Dissipative interactions have been approached by means of phenomenological models based on the relaxation time approximation, [11–13] and also by introducing an actual Boltzmann-like collision operator [10, 14]. The phonon collision operator acting upon the Wigner function has been initially suggested as an *a priory* assumption that 'is an adequate approximation at some level' [10]. The model, that accounts for the action of both, the quantum potential operator V_w and the classical scattering operator $\mathcal{B}$ is now called Wigner-Boltzmann (WB) equation

$$\frac{\partial f_w(x,\mathbf{k},t)}{\partial t} + \frac{\hbar k_x}{m}\frac{\partial}{\partial x}f_w(x,\mathbf{k},t)$$

$$= \int dk'_x\, V_w(x, k_x - k'_x)\, f_w(x, k'_x, \mathbf{k}_{yz}, t) + \mathcal{B} f_w(x, \mathbf{k}', t), \quad (4)$$

$$\mathcal{B} f_w(x, \mathbf{k}', t) = \int d\mathbf{k}'\, f_w(x, \mathbf{k}', t) S(\mathbf{k}', \mathbf{k}) - f_w(x, \mathbf{k}, t)\lambda(\mathbf{k}).$$

The two components of $\mathcal{B}$ are $S(\mathbf{k}, \mathbf{k}')$—the scattering rate for a transition from $\mathbf{k}$ to $\mathbf{k}'$, and $\lambda(\mathbf{k}) = \int d\mathbf{k}'\, S(\mathbf{k}, \mathbf{k}')$, the total out-scattering rate. We note that even a one-dimensional problem involves the complete 3D wave vector space.

The equation has been derived from first principles only recently for interactions with ionized impurities [15] and with phonons [16]. The two approaches are very different and involve a set of assumptions and approximations: a large number of dopant atoms, a fast collision approximation, a weak scattering limit and an equilibrium phonon system. These assumptions require that the dwell time of the carriers inside the device, and hence the device itself, must be sufficiently large. On the contrary, the application of the Wigner potential operator is reasonable in small domains, where the potential changes over a region comparable with the coherence length of the electron. Thus the WB equation is expected to be relevant for devices composed by active quantum domain(s) embedded into large classical regions.

The WB equation may become a basic model for understanding nano-device behavior. Recent studies of ultra-small double-gate MOSFET demonstrate that the equation successfully fills the gap between purely coherent transport and the classical Boltzmann model and allows to establish a seamless link between classical and quantum transport regions [7]. Beyond the analysis of direct source-drain tunneling and quantum reflections on the steep potential drop at the drain-end of the channel, the results emphasize the role of scattering which remains surprisingly important [17] in such a small device in spite of significant quantum coherence effects. The theory of decoherence has shown that a semi-classical behavior may emerge from the interaction with the environment. For electrons in nanodevices the mechanism which may induce such behavior is interaction with phonons and defects [18].

2.3 Scattering-induced Wigner correction

Important for device modeling is the stationary problem, determined by boundary conditions. Nondegenerate boundaries are characterized by the Maxwell-Boltzmann (MB) distribution with the Fermi energy as a parameter. Equation (4) requires a MB distribution in the full 3D wave vector space. The coherent task usually relies on a reduction of the dimensions via an integration over the transversal wave vector components $\mathbf{k}_{yz}$. Alternatively, the present approach utilizes the fact that the solution of (2) can be augmented by a $\mathbf{k}_{yz}$ dependence, which remains arbitrary unless specified from the boundaries. Hence, a MB distribution $f_{MB}(k'_{yz})$ is assumed in the yz directions, and the functions

$$f_w^c(x, \mathbf{k}') = f_w^c(x, k'_x) \frac{\hbar^2}{2\pi mkT} e^{-\frac{\hbar^2(k'^2_y + k'^2_z)}{2mkT}};$$

$$f_w^\Delta(x, \mathbf{k}) = f_w(x, \mathbf{k}) - f_w^c(x, \mathbf{k})$$

can be introduced. The coherent solution f_w^c is assumed as known in what follows, calculated e.g. by some of the existing coherent approaches. The scattering induced Wigner correction equation (SIWCE) for f_w^Δ is obtained by subtracting the coherent counterpart from (4).

$$\frac{\hbar k_x}{m} \frac{\partial}{\partial x} f_w^\Delta(x, \mathbf{k}) = \int dk'_x\, V_w(x, k'_x - k_x) f_w^\Delta(x, k'_x, \mathbf{k}_{yz}) + \mathcal{B} f_w^\Delta(x, \mathbf{k}') + f_w^{\Delta 0}, \quad (5)$$

$$f_w^{\Delta 0} = \int d\mathbf{k}'\, f_w^c(x, \mathbf{k}') S(\mathbf{k}', \mathbf{k}) - f_w^c(x, \mathbf{k})\lambda(\mathbf{k}).$$

This model has several peculiarities: It resembles the WB equation with an additional free term $f_w^{\Delta 0} = \mathcal{B} f_w^c$, which is the first iteration of the Boltzmann scattering operator on the known coherent solution. The latter provides an initial condition, whose evolution is directed from the internal part of the device towards the boundaries. The conditions there are modified by the fact that the correction is zero at the boundaries: only their absorbing properties remain, no carriers are injected into the device. So far no approximations are introduced, the SIWCE is fully equivalent to (4). However, as the information about the coherent behavior is already available, some approximations may be afforded in (5).

First, the smooth part of the potential may be separated into a classical force as discussed in the next section. Second the rest of the potential, used for the operator V_w may be gradually eliminated in the limit $L_{coh} \to 0$. This operator is the main cause for the numerical burden for particle approaches to the WB equation. Thus a numerically feasible model can be adjusted by a proper choice of L_{coh}. The limit corresponds to a purely classical Boltzmann evolution of an initial condition towards the absorbing boundaries. The latter also work in favour of the numerical convergence. Indeed, carrier transport in small devices is close to ballistic, so that already the term $f_w^{\Delta 0}$, may be close enough to the full solution. However, the classical limit is justified only for smooth potentials, as will be shown in the last section, (13).

3 Numerical particle methods

The first numerical applications of the coherent Wigner approach are based on deterministic methods [11, 19], further refined towards self-consistent schemes with the Poisson equation. One of the main problems of these methods

is related to the discretization of the diffusion term because of the typically rapid variations of the Wigner function. In some cases the discretization scheme may influence the simulated device characteristics [20–22]. Moreover, an application to multi-dimensional devices is prohibited by the enormous increase of the memory requirements.

Stochastic, or particle methods may overcome the memory requirements and can naturally incorporate the carrier scattering inherent for the Wigner-Boltzmann equation. Particle approaches benefit from all the knowledge acquired for years in semi-classical device modeling and especially in the physics of carrier scattering. The major challenge for such methods is to account for the negative values of the quasi-distribution caused by the Wigner potential. It has been solved by two particle approaches, with rather different heuristic interpretation aiming to give simulated particles the property to carry negative contributions. The first one describes the Wigner function as a sum of Dirac excitations still localized in the phase-space but weighted by an amplitude, called affinity in [23, 24]. The particle affinities contain all the information on the quantum state of the electron system. They evolve continuously along classical Newton trajectories and account for the local values of the Wigner potential via the affinities, which thus can take negative values. The affinities carried by the particles are taken into account as weights in the reconstruction of the Wigner function and in the computation of all physical averages.

The second approach interpretes the Wigner equation, with a Boltzmann scattering term as a Boltzmann equation with a generation term [25]. The interaction with the Wigner potential gives rise to generation of particle pairs with opposite sign. The sign is the basic property which outlines the introduced numerical particles from classical quasi-particles. It is an important property, since positive and negative particles can annihilate one another. The negative values of the Wigner function in certain phase space regions can be explained in a natural way by the accumulation of negative particles in these regions. The Wigner-Boltzmann transport process corresponds to drift, scattering, generation and annihilation of these particles.

These models present the state of the art in the field and unify classical and quantum regions within a single transport picture where the scattering occurs in the full wave vector space. Two dimensional devices can be considered [26–28].

The same principles can be, but are not yet, applied to (5) for developing a Monte Carlo model. Such an approach has been developed only for the evaluation of $f_w^{\Delta 0}$, and provides a picture where evolving Boltzmann particles accumulate weight λ'/λ, which is the ratio of the total out-scattering rates at the beginning and at the end of the free flights [29].

In all these approaches particles are accelerated by a local classical force obtained by separation of the potential into classical and quantum components. It completes the left hand sides of (2), (4) and (5) to the general form of the Liouville operator. A way for such separation is suggested in the next section, where the coherent problem is considered for convenience.

4 Wigner potential and classical force

The Fourier transform $\tilde{V}(q)$ of the potential $V(x)$ can be expressed in polar form by its modulus and phase.

$$\begin{aligned}\tilde{V}(q) &= \int dx\, V(x) e^{-iqx},\\ V(x) &= \frac{1}{2\pi}\int dq\, \tilde{V}(q) e^{iqx},\\ \tilde{V}(q) &= A(q) e^{i\varphi(q)}.\end{aligned} \tag{6}$$

With the variable substitutions $s = x \pm x'/2$ the integrals in the definition (3) of the Wigner potential can be evaluated as

$$\begin{aligned}\int dx'\, V\left(x+\frac{x'}{2}\right) e^{-ikx'} &= 2e^{2ikx}\tilde{V}(2k);\\ \int dx'\, V\left(x-\frac{x'}{2}\right) e^{-ikx'} &= \left[2e^{2ikx}\tilde{V}(2k)\right]^*,\end{aligned} \tag{7}$$

and the following relation can be established.

$$\begin{aligned}V_w(x,k) &= \frac{1}{i\hbar(2\pi)}\left\{2e^{2ikx}\tilde{V}(2k) - \left[2e^{2ikx}\tilde{V}(2k)\right]^*\right\}\\ &= \frac{2}{\pi\hbar}A(2k)\sin[\varphi(2k)+2kx]\end{aligned}$$

where the polar form (6) has been used. The x-dependence of the Wigner potential is given analytically by an undamped sine function, independent of the actual shape of the potential. This result also shows, that even for a well localized potential barrier the Wigner potential is fully de-localized in the coordinate space. In any numerical procedure, therefore, the Wigner potential needs to be truncated at some finite x-coordinate.

The function $\Delta(x,x') = V(x+\frac{x'}{2}) - V(x-\frac{x'}{2})$ is an odd function with respect to x': $\Delta(x,-x') = -\Delta(x,x')$ Due to this antisymmetry, the substitution $\exp(-ikx') = \cos(kx') - i\sin(kx')$ in (3) readily yields the Fourier sine transform.

$$V_w(x,k) = -\frac{1}{\hbar(2\pi)}\int \mathrm{d}x'\, \Delta(x,x')\sin(kx'). \tag{8}$$

In general the potential $V(x)$ is given within a finite simulation domain, representing, for instance, the active region of an electronic device. Outside of this domain the potential is continued by two constants, say V_L and V_R. This situation represents an active device region connected to semi-infinite leads on both sides, where the leads are assumed to be

ideal conductors. Therefore, in practical cases Δ will have the asymptotic behavior, $\lim_{x'\to\pm\infty}\Delta(x,x') = \mp(V_L - V_R)$ where $(V_L - V_R)$ is the potential difference between the left and the right lead. Since the integrand in (8) does not vanish at infinity, the Fourier integral will diverge at $q = 0$. From the asymptotic behavior of $\Delta(x,x')$ for $x' \to \infty$ we find the asymptotic behavior of $V_w(x,k)$ for $k \to 0$.

$$\begin{aligned}\Delta(x,x') &\simeq (V_R - V_L)\mathrm{sgn}(x'), \quad x' \to \infty \\ V_w(x,k) &\simeq= \frac{2(V_L - V_R)}{\hbar(2\pi)}\mathcal{P}\frac{1}{k}, \quad k \to 0.\end{aligned} \tag{9}$$

Here, sgn denotes the signum function and $\mathcal{P}$ the principal value. This consideration shows that if the potential difference is nonzero, there will be a pole in the Wigner potential at $k = 0$. Numerical methods for the Wigner equation generally use a k-space discretization, where the discrete k-points are located symmetrically around the origin and the point $k = 0$ is not included. In this way, no particular treatment of the singularity is needed.

To deal with the singularity of V_w, one can define a small neighborhood around $q = 0$ and split the domain of integration as follows [30].

$$\begin{aligned}Qf_w(x,k) &= \int dq\, V_w(x,q) f_w(x,k-q) \\ &= \int_{|q|\le q_c/2} + \int_{|q|>q_c/2} \\ &= Q_{cl} f_w + Q_{qm} f_w.\end{aligned} \tag{10}$$

Here q_c is some small wave number. In this way, we have split the potential operator Q in two parts, which we refer to as Q_{cl} and Q_{qm}. A linearization can be introduced in the integral over the small wave numbers.

$$Q_{cl} f_w(x,k) = -\frac{\partial f_w(x,k)}{\partial k} \int\limits_{|q|\le q_c/2} dq\, q V_w(x,q) \tag{11}$$

with

$$\begin{aligned}-\int\limits_{|q|\le q_c/2} dq\, q V_w(x,q) &= \frac{\partial}{\partial x}\Re\left\{\frac{1}{2\pi\hbar}\int_{-q_c}^{q_c} dq\, \tilde{V}(q) e^{iqx}\right\} \\ &= \frac{1}{\hbar}\frac{\partial}{\partial x} V_{cl}(x).\end{aligned} \tag{12}$$

Here we introduced the classical potential component, which is a real function:

$$\begin{aligned}V_{cl}(x) &= \frac{1}{2\pi}\int_{-q_c}^{q_c} dq\, \tilde{V}(q) \mathrm{e}^{iqx} \\ &= \frac{1}{2\pi}\int_{-q_c}^{q_c} dq \int dy\, V(y) e^{iq(x-y)} \\ &= \int dy\, V(y) \frac{\sin[q_c(x-y)]}{\pi(x-y)}.\end{aligned} \tag{13}$$

The classical potential component shows a smooth spatial variation, as it is composed of long-wavelength Fourier components only. Equation (13) motivates the following spectral decomposition of the potential profile into a slowly varying, classical component (13) and a rapidly varying, quantum mechanical component.

$$V(x) = V_{cl}(x) + V_{qm}(x). \tag{14}$$

The two potential components have the following properties. The classical component accommodates the applied voltage. As it is treated through a classical force term, it does not induce any quantum reflections. The quantum mechanical component vanishes at infinity and has a smooth Fourier transform.

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