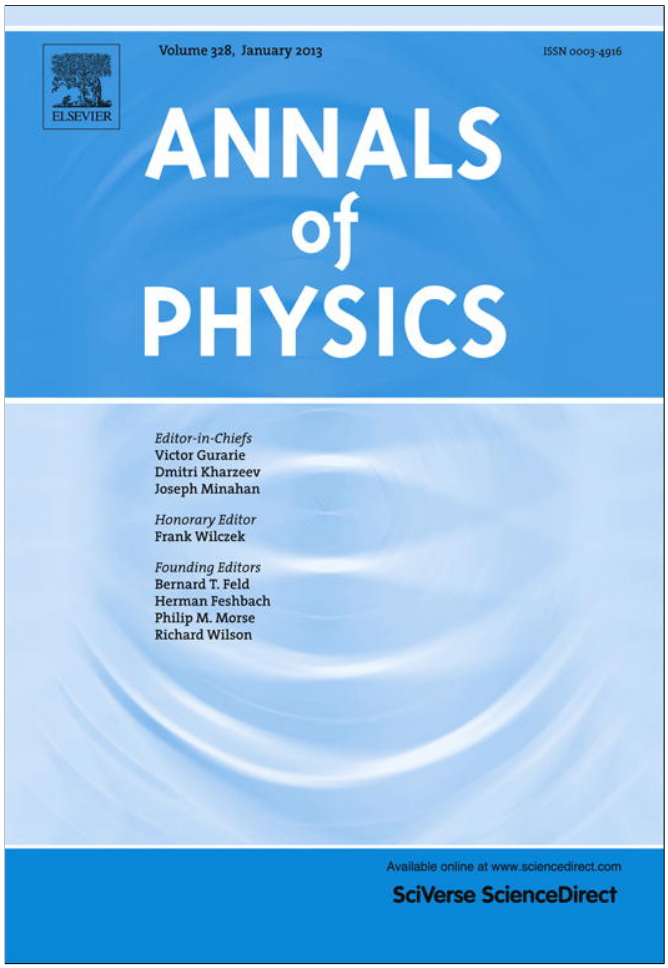

Annals of Physics 328 (2013) 220–237

Contents lists available at SciVerse ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

Physical scales in the Wigner–Boltzmann equation

M. Nedjalkov [a,*], S. Selberherr [a], D.K. Ferry [b], D. Vasileska [b], P. Dollfus [c], D. Querlioz [c], I. Dimov [d], P. Schwaha [e]

[a] Institute for Microelectronics, Vienna University of Technology, Vienna, Austria
[b] Department of Electrical Engineering, Arizona State University, Tempe, AZ, USA
[c] Institute of Fundamental Electronics, CNRS, University of Paris-sud, Orsay, France
[d] Institute for IC Technology, Bulgarian Academy of Sciences, Sofia, Bulgaria
[e] Shenteq s.r.o., Bratislava, Slovak Republic

ARTICLE INFO

Article history:
Received 14 May 2012
Accepted 2 October 2012
Available online 9 October 2012

Keywords:
Wigner–Boltzmann equation
Quantum transport
Decoherence
Scattering

ABSTRACT

The Wigner–Boltzmann equation provides the Wigner single particle theory with interactions with bosonic degrees of freedom associated with harmonic oscillators, such as phonons in solids. Quantum evolution is an interplay of two transport modes, corresponding to the common coherent particle-potential processes, or to the decoherence causing scattering due to the oscillators. Which evolution mode will dominate depends on the scales of the involved physical quantities. A dimensionless formulation of the Wigner–Boltzmann equation is obtained, where these scales appear as dimensionless strength parameters. A notion called scaling theorem is derived, linking the strength parameters to the coupling with the oscillators. It is shown that an increase of this coupling is equivalent to a reduction of both the strength of the electric potential, and the coherence length. Secondly, the existence of classes of physically different, but mathematically equivalent setups of the Wigner–Boltzmann evolution is demonstrated.

1. Introduction

The Wigner theory establishes a phase space formulation of quantum mechanics, where both states and observables are represented by functions of coordinates and momenta. Many notions of classical

* Correspondence to: Institute for Microelectronics, Vienna University of Technology, Gußhausstraße 27-29/E360, A-1040 Vienna, Austria. Tel.: +43 158801 36044; fax: +43 158801 36099.
E-mail address: mixi@iue.tuwien.ac.at (M. Nedjalkov).

0003-4916/$ – see front matter © 2012 Elsevier Inc. All rights reserved.
doi:10.1016/j.aop.2012.10.001

statistical mechanics such as probability distributions and mean values are retained in this picture, which recovers physical intuition in the field of quantum theory. Historically introduced with the help of the Schrödinger equation [1,2], modern Wigner theory represents an independent formulation, recognized as equivalent and autonomous alternative to operator mechanics [3]. The formalism has been further applied to scattering problems within the basic particle–potential interaction, and beyond, to multiple scattering problems [4]. With the introduction of additional degrees of freedom, which need to be eliminated by corresponding averaging, the single particle state ceases to be pure, so that irreversibility and effects of decoherence begin to characterize the evolution of the particle state.

The problem of environmentally induced decoherence of quantum systems to semi-classical states has been a subject of intensive research over the past three decades [5,6]. In particular, the concept of einselection of pointer states has been very successful in explaining the general behavior of quantum particles subjected to decoherence effects both from a fundamental point of view [7,8] and in solid-state nanostructures such as open quantum dots [9]. The Wigner function is recognized as a convenient formalism to study these processes theoretically [8,10], or experimentally [11]. Recently, the application of quantum physics to information theory has enlarged the interest in sources and time scales of decoherence processes as part of the efforts to develop devices for quantum processing of signals. Decoherence effects may even have a strong influence on the behavior of more conventional nanoscaled solid-sate devices [12]. In this field the Wigner formalism is nominated as a legitimate inheritor of the classical solid-state electron transport model, as it provides an extension of the latter for kinetic processes occurring in nanoscale devices [13], which is demonstrated by simulations of a variety of transport conditions in actual devices like RTD's and DG-MOSFET's [14] and of the scattering-induced decoherence in semiconducting nanostructures [15].

In this way the problem of exploring the gap between quantum–coherent and scattering dominated evolution modes has both fundamental and practical aspects. The physical system chosen for this purpose presents solid state electrons moving in a given electric field and interacting with lattice vibrations, described in terms of harmonic oscillators—phonons. While the approach applied in the following remains general, the concrete system allows to regard phonons as a thermostat—an environment which causes decoherence without being affected by the electron subsystem. This allows to perform averaging and to obtain the Wigner–Boltzmann (WB) equation for the electrons where the environment participates with well-defined Bose equilibrium averages.

The fundamentals of the equation can be traced back to certain uniform field transport models, which utilize the Wigner formalism to derive classical [16], or quantum-mechanical [17] electron–phonon interaction operators. The Wigner equation augmented by a Boltzmann-like collision operator has been suggested for the case of general potentials as an intuitive deduction from these models [18–20] It has been demonstrated that phase-breaking and energy dissipation processes are needed to maintain the physical behavior of the modeled system [21,22] Thus, initially, the Boltzmann-like phonon collision operator acting upon the Wigner quasi-distribution is an a priori, but necessary assumption that 'is an adequate approximation at some level' [21]. What are the physical conditions allowing the common existence of the classical scattering operator next to the quantum Wigner-potential operator? The answer is not trivial: derivations from first principles and analysis of the assumptions and approximations have been provided only recently for interactions with ionized impurities [23] and with phonons [24]. Relations between spatial, energy and time scales are specified by theories which turn out to be relevant to the transport conditions in modern nanoelectronic devices.

As implied by the name of the Wigner–Boltzmann equation, the two limiting regimes of coherent or classical transport are obtained by setting one of the corresponding operators to zero. They have rather opposing roles in determining the properties of the solution.

If the coupling with the phonons becomes negligible, two different situations may occur. If the electric potential changes up to quadratically within the spatial extension of the electron wave packet, the electron is a particle with a ballistic evolution along classical Newton's trajectories. Otherwise the kinetics are quantum–coherent. The electric potential causes oscillations and negative values, around abrupt potential changes in regions of tunneling and quantization [25]. These features are the manifestations of the quantum character of the Wigner function even for the simple situation of an initial state resulting from a superposition of two Gaussian wave functions [5]. In this case, oscillations

and negative values demonstrate an entangled pure state. If they are removed, the state obtained has a completely different physical meaning: it is a mixed state determined by the probabilities of the electron to be in one or the other sub-states related to the two wave functions.

With scattering processes enabled, the Boltzmann operator strives to modify the electron state, until the thermal equilibrium distribution is obtained. It destroys, in this way, the coherent properties of the solution introducing irreversibility and a classical probability picture. Depending again on the way the potential changes, the transport is classical, of Boltzmann type, if the field is slowly varying. Otherwise it corresponds to a mixed mode, comprised by coherent electron–potential interaction along with decoherence due to electron–lattice interaction, as described by the general form of the WB equation.

Apparently, the physical scales involved determine which one of these two adversely acting operators dominates the transport regime. The distinction between quantum and classical behavior is the focus of this paper, it is measured by the difference in the corresponding expectation values of the observables. We investigate the role of relevant scaling parameters on this difference.

The paper is organized as follows. The needed concepts and notions, devoted to coherent evolution, are introduced in the first part. Operator mechanics provide the classical limit of the dynamics of a given physical observable by formally letting $\hbar \to 0$. In this case the commutator $[\cdot,\cdot]_-$ reduces to the Poisson bracket $[\cdot,\cdot]_P$ which determines the evolution of the dynamical functions of the classical mechanics. A quantity ϵ, which is called the semiclassical parameter, and varies in accordance to the scales involved, effectively replaces $\hbar$ in a scaled Schrödinger equation. The difference between the classical and quantum evolution of a given physical quantity goes to zero corresponding to ϵ^2, as evaluated by an inference, known in the mathematical literature as Egorov's theorem [26,27]. The same concept is alternatively formulated in phase space with the purpose of applying it to the analysis of mixed mode processes. We first obtain a convenient dimensionless formulation of the coherent Wigner theory in terms of ϵ. A condition is found, such that ϵ appears as a counterpart of $\hbar$ in well known interrelations of standard theory. The Egorov theorem is then generalized for the mixed mode WB evolution which is then considered in the Section 3. The involved physical scales are those of the device potential, the phonon energy, and the electron–phonon coupling. Dimensionless parameters corresponding to the relative strength of these quantities are introduced in the scaled electron–phonon Schrödinger equation. The latter is the ancestor of the scaled Wigner–Boltzmann equation, whose derivation focuses on the appearance of these parameters in the components of the kernel of the equation. It is shown that the increase of the electron–phonon coupling leads to a super-linear decrease of the quantum contribution due to a decrease of both, the proportion of the coherent component and the semiclassical parameter ϵ. This result is formulated by the scaling theorem which gives physical insight to the involved processes causing classical behavior. This analysis shows that two factors are primarily responsible: the first one is related to the strength of the scattering processes, and the second one, as implied by Egorov's theorem, is due to the scattering-induced reduction of the coherence length. In the end we demonstrate by virtue of applying the scaling theorem the existence of systems which are physically very different, however, result in mathematically equivalent evolution. This is supported by numerical experiments demonstrating the evolution of entangled electron states. Typical semiconductor transport scales are discussed in the Appendix A to provide a range of values for ϵ.

2. Coherent evolution

2.1. Wave mechanics and Egorov's theorem

This section introduces the dimensionless Schrödinger equation, and the basic notions of quantum and classical evolution of mean values of physical observables needed to estimate their difference by the Egorov theorem.

2.1.1. Dimensionless Schrödinger equation

The time dependent Schrödinger equation for a particle in a potential $V(X)$ describes its evolution from an initial condition Ψ_0.

$$i\hbar\frac{\partial\Psi(X,T)}{\partial T} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial X^2}\Psi(X,T) + V(X)\Psi(X,T). \tag{1}$$

(While the current development is in one dimension only, the results are easily extended to higher dimensions, and we will turn to the vector form later in the paper.) The physical scales involve distance, energy, and time: $X = Lx$, $V(Lx) = V_0 v(x)$, $T = T_0 t$. Moreover, only two can be independent, which offers different sets of choices. A natural set of scaling factors is suggested in Appendix A. Currently we continue with the following selection: Principal physical quantities are L, and V_0, and they determine the time units $T_0 = \sqrt{\frac{m}{V}_0} L$ (which we discuss further below). This allows us to introduce the quantity

$$\epsilon = \frac{\hbar}{T_0 V_0} = \sqrt{\frac{\hbar^2}{mL^2 V_0}}, \tag{2}$$

and to scale the equation as:

$$i\epsilon \frac{\partial \psi^\epsilon(x,t)}{\partial t} = -\frac{\epsilon^2}{2}\frac{\partial^2}{\partial x^2}\psi^\epsilon(x,t) + v(x)\psi^\epsilon(x,t). \tag{3}$$

All quantities ϵ, x, t, $v(x)$ are now dimensionless variables.

We need to compare the classical and quantum laws giving the evolution of the physical observables. Physical quantities are defined in classical mechanics by dynamical functions of particle position and momentum. Wave mechanics associates operators acting in the Hilbert space spanned by the solutions of the Schrödinger equation. We recall the needed basic concepts of these two theories.

2.1.2. Classical observables

The classical phase space is defined by the Cartesian product of the particle position x and momentum p. Physical quantities are dynamical functions $A(x, p)$, which we consider depending on the phase space coordinates but not explicitly on the time, such as the kinetic and potential energies and their sum giving the Hamiltonian $H(x, p)$. The state of the a single particle at a given time is presented by a point in the phase space. Provided that the initial particle coordinates x, p are known, the novel coordinates $x(t), p(t)$ at time t are obtained from the Hamilton equations. Let us consider the function $A(t)$ that describes the evolution of a generic physical quantity A. Since the laws of mechanics do not change with time, A remains the same function for the old and the new coordinates, $A(t) = A(x(t), p(t))$. Then the Hamilton equations allow to introduce the Poisson bracket $[\cdot,\cdot]_P$ and the equation of motion of $A : \dot{A} = [A, H]_P$, $[x, p]_P = 1$. The Poisson bracket $[\cdot,\cdot]_P$, gives rise to an automorphic (conserving the algebraic structure) mapping of the set of the dynamical functions. Indeed, as these are assumed 'good' enough to be presented as polynomials, i.e. by algebraic operations, this mapping takes the form:

$$\sum A_{ij} x^i p^j \to \sum A_{ij} x(t)^i p(t)^j = \sum A_{ij}(t) x^i p^j$$

or

$$A(x, p) \to A(t, x, p) = A\left(x(t), p(t)\right). \tag{4}$$

Eq. (4) introduces the new function of the old coordinates $A(t, x, p)$. It is a classical analog of the equivalence between Heisenberg and Schrödinger representations of wave mechanics. This property and its quantum-mechanical counterpart are needed for the application of Egorov's theorem. The operator structure of the wave mechanics can be introduced with the help of the correspondence principle.

2.1.3. Quantum-mechanical observables

According to this principle, classical position and momentum variables correspond to the Hermitian operators $\hat{x}$ and $\hat{p}$ satisfying a quantum mechanical counterpart of the Poisson bracket:

$$x \to \hat{x} \qquad p \to \hat{p} \qquad \hat{x}\hat{p} - \hat{p}\hat{x} = [\hat{x}, \hat{p}]_- = i\epsilon\hat{1}. \tag{5}$$

We note that the ϵ based quantum dynamics are in correspondence with the dimensionless Eq. (3), where the momentum operator in the position representation is $p = -i\epsilon\partial/\partial x$.

The operators $\hat{A}$ of wave mechanics are defined with the help of this correspondence

$$A(x,p) = \sum A_{ij}x^i p^j \rightarrow \sum A_{ij}\hat{x}^i\hat{p}^j = A(\hat{x},\hat{p}) = \hat{A}. \tag{6}$$

The evolution equation and the expectation value of the physical observable A in state ψ is given by:

$$i\epsilon\dot{\hat{A}} = [\hat{A},\hat{H}]_- \qquad \langle A\rangle(t) = \langle\psi|\hat{A}|\psi\rangle. \tag{7}$$

The commutator in the first relation gives an automorphic mapping in time of the operators: $\hat{A}(t,\hat{x},\hat{p}) = \hat{A}(\hat{x}(t),\hat{p}(t))$ exactly as in the classical case, Eq. (4). The rule (6) is ambiguous until a specification of the operator ordering is given, which is provided by the fully symmetrizing Weyl correspondence:

$$\begin{aligned}\hat{A} &= \hat{A}(\hat{x},\hat{p}) = \int dsdq\beta(s,q)e^{i(s\hat{x}+q\hat{p})};\\ \beta(s,q) &= \frac{1}{(2\pi)^2}\int dxdpA(x,p)e^{-i(sx+qp)}.\end{aligned} \tag{8}$$

Here β is adjoined to the *function* A via the Fourier transform. The Weyl transform establishes a one-to-one correspondence between phase space functions and operators. From this definition one can express the action of an operator $\hat{A}$ on the state function $|\psi\rangle$ with the help of the function $A(x,p)$.

We complete the introduction of the notions needed for evaluation of the desired difference of the expectation values by considering the operators obtained in the following two ways:

$$\begin{aligned}A(x,p) &\overset{\text{Weyl}}{\leftrightarrow} \hat{A}(\hat{x},\hat{p}) \overset{\hat{x}(t),\hat{p}(t)\text{via}[\cdot,\cdot]_-}{\longrightarrow} \hat{A}(\hat{x}(t),\hat{p}(t)) = \hat{A}(t,\hat{x},\hat{p})\\ &\neq \quad A(x,p) \overset{x(t),p(t)\text{via}[\cdot,\cdot]_P}{\longrightarrow} A_P(x(t),p(t)) = A_P(t,x,p) \overset{\text{Weyl}}{\leftrightarrow} \hat{A}_P(t,\hat{x},\hat{p}).\end{aligned} \tag{9}$$

According to the first row, the operator $A(\hat{x},\hat{p})$ is obtained at time 0 from the dynamical function $A(x,p)$ via the Weyl transform, and then is evolved until time t quantum mechanically, with the help of the commutator $[\cdot,\cdot]_-$. This procedure gives rise to the operator $\hat{A}(t)$. In the second mapping the arguments x and p of $A(x,p)$ are first evolved until time t via the Poisson bracket $[\cdot,\cdot]_P$, giving rise to the function $A_P(x(t),p(t))$. The next equality shows how this function is interpreted in the Weyl transform: via Eq. (8) it gives rise to the image $\beta_P(t,s,q)$, which is used to obtain the operator $\hat{A}_p(t,\hat{x},\hat{p})$.

Egorov's theorem applied to these particular operators links them into an equality, which can be approximated to an estimate of the difference between the corresponding expectation values in a state $|\psi^\epsilon(t)\rangle = e^{i\hat{H}^\epsilon t/\epsilon}|\psi_0\rangle$ which is the solution of Eq. (3) for an initial condition $|\psi_0\rangle$:

$$\langle A\rangle(t) = \langle\psi_0|\hat{A}(t)|\psi_0\rangle = \langle\psi^\epsilon(t)|\hat{A}|\psi^\epsilon(t)\rangle = \langle\psi_0|\hat{A}_P(t,\hat{x},\hat{p})|\psi_0\rangle + O(\epsilon^2). \tag{10}$$

The first two terms correspond to Heisenberg and Schrödinger pictures, while the third one to a classical evolution.

The following important result, which can be called $E\epsilon$-estimate is further derived: $O(\epsilon^2) = M\epsilon^2 t$, with M a constant and t the evolution time [28]. This result gives an answer to the question of how long the classical and quantum evolutions stay close, within a prescribed error, and is evaluated for a time interval with a maximal duration of order $-\log(\epsilon)$, called the Ehrenfest time [29].

In the following we show how Eq. (10) and the $E\epsilon$-estimate can be derived in terms of classical and quantum (quasi) distribution functions. The latter re-establish the phase space as a common concept for classical and quantum notions. We pursue the idea to first derive the corresponding dimensionless evolution equations, and then to investigate their difference.

2.2. Phase space reformulation

2.2.1. Dimensionless Wigner function

The starting entity is the density matrix ρ^ϵ, which is introduced if Definition (7) is rewritten as:

$$\langle A\rangle(t) = \int dx' \langle x'|\hat{A}(\hat{x},\hat{p})|\psi^\epsilon(t)\rangle\langle\psi^\epsilon(t)|x'\rangle; \qquad \rho^\epsilon(x,x',t) = \langle x|\psi^\epsilon(t)\rangle\langle\psi^\epsilon(t)|x'\rangle. \tag{11}$$

The Wigner function is obtained by the Fourier transform of ρ^ϵ. The most general form of the dimensionless Fourier transform introduces another, arbitrary constant ϵ':

$$f_w^{\epsilon,\epsilon'}(x,p,t) = \int \frac{dx'}{(2\pi\epsilon')} e^{-i\frac{x'p}{\epsilon'}} \rho^\epsilon\left(x+\frac{x'}{2}, x-\frac{x'}{2}, t\right), \tag{12}$$

ϵ' may be determined by imposing some physical criterion, which here is chosen heuristically: we wish, if possible, to have a function (12) which recovers the classical way of obtaining averages:

$$\langle\hat{A}\rangle(t) = \int dxdpA(x,p) f_w^{\epsilon,?}(x,p,t).$$

Lengthy calculations, involving (11) and (8) show that this is possible, and gives rise to the condition $\epsilon' = \epsilon$. It is thus sufficient to retain a single superscript in the notation for the dimensionless Wigner function.

In this way, the problem for finding $\langle A\rangle(t)$ is replaced by the problem for finding f_w^ϵ. The equation of motion for f_w^ϵ is derived with the help of the dimensionless Schrödinger equation (3) and Definition (12), along with $\epsilon' = \epsilon$.

2.2.2. Dimensionless Wigner equation

Formal derivations give rise to the following relations:

$$\frac{\partial f_w^\epsilon(x,p,t)}{\partial t} + p\frac{\partial f_w^\epsilon(x,p,t)}{\partial x} = \int dp' v_w^\epsilon(x,p-p') f_w^\epsilon(x,p',t), \tag{13}$$

$$v_w^\epsilon(x,p) = \frac{1}{i\epsilon 2\pi\epsilon}\int dx' e^{-ix'p/\epsilon}(v(x+x'/2) - v(x-x'/2)), \tag{14}$$

for the Wigner function and the Wigner potential, where all arguments are dimensionless quantities. A comparison of these expressions with the standard definitions shows that ϵ replaces $\hbar$ everywhere. This is very convenient since (i) all derived formulas and notions of the Wigner theory can be reused by just exchanging the two constants; (ii) it gives rise to the consistency criteria $X \to x, P \to p, \hbar \to \epsilon$ allowing to determine the scaling factors P_0 and K_0 of the dimensionless counterparts p and k of momentum and wave vector:

$$p = \frac{\epsilon}{x}; \qquad P_0 = \frac{T_0 V_0}{L}; \qquad K_0 = \frac{1}{L\epsilon}. \tag{15}$$

In order to compare Eq. (13) with its classical counterpart, we need to formulate the latter in terms of x and p.

2.2.3. Collisionless Boltzmann equation

The obtained dimensionless ballistic Boltzmann equation is:

$$\frac{\partial f(x,p,t)}{\partial t} + p\frac{\partial f(x,p,t)}{\partial x} + \phi(x)\frac{\partial f(x,p,t)}{\partial p} = 0 \quad \phi(x) = -\frac{\partial v(x)}{\partial x}. \tag{16}$$

We note the absence of any explicit dependence on ϵ. Any real differentiable function of the phase space can be a solution of (16). Distribution functions obey the restriction of having non-negative values, which is introduced by considerations about the probabilistic meaning of the initial condition. As an aside, we note that some authors smooth the Wigner distribution with a Gaussian to remove these negative parts, and this leads to the so-called Husumi distribution [30]. However, this restriction is not imposed here: quasi-distributions may be solutions, regarded as linear combinations of distributions.

2.2.4. Pure state quantum correction f^{Δ}

The approach suggested below is an alternative to the idea of the Scattering Induced Wigner Correction Equation (SIWCE) [31,32]. The latter describes the evolution of a quantity, obtained by the difference of the two solutions, corresponding to coherent and mixed mode transport. Alternatively a truncated Wigner approximation and quantum corrections around the classical limit are recently discussed in [33]. Accordingly, here we investigate the evolution of the difference between the ballistic quantum and classical regimes of transport, described by the quantum correction $f^{\Delta} = f_w^{\epsilon} - f$.

The Taylor expansion of the potential difference in (14) contains only odd terms:

$$v_w^{\epsilon}(x,p) = \frac{1}{i\epsilon 2\pi\epsilon}\int dx' e^{-ix'p/\epsilon}\sum_{n=0}^{\infty}\frac{2}{(2n+1)!}\frac{d^{(2n+1)}v(x)}{dx^{(2n+1)}}\left(\frac{x'}{2}\right)^{(2n+1)}. \tag{17}$$

The contribution of the first, $n = 0$, term $v_{w,0}^{\epsilon}$ to the Wigner equation is:

$$\int dp' v_{w,0}^{\epsilon}(x,p-p')f_w^{\epsilon}(x,p',t) = -\phi(x)\frac{f_w^{\epsilon}(x,p,t)}{\partial p}. \tag{18}$$

Transferred to the left this term completes the left hand side of (13), which becomes equivalent to (16). This suggests to subtract (16) from (13), which gives rise to an integro-differential equation with the complete Liouville operator $\mathcal{L}$ acting on the function $f^{\Delta} = f_w^{\epsilon} - f$, and an integral operator $\tilde{\mathcal{V}}_w^{\epsilon}$ to the right: $\mathcal{L}f^{\Delta} = \tilde{\mathcal{V}}_w^{\epsilon}f_w^{\epsilon}$ whose kernel $\tilde{v}_w^{\epsilon}$ differs from v_w^{ϵ} in (17) only by the missing term $n = 0$. It is convenient to continue with the integral form of the equation, which is obtained with the help of the Newton's trajectories $X(t')$, $P(t')$ initialized by x, p, t, which define the inverse $\mathcal{L}^{-1}$ of the Liouville operator [34]:

$$f^{\Delta}(x,p,t) = \mathcal{L}^{-1}\tilde{\mathcal{V}}_w^{\epsilon}f_w^{\epsilon} = \int_0^t dt'\int dp'\tilde{v}_w^{\epsilon}(X(t'),P(t')-p')f_w^{\epsilon}(X(t'),p',t). \tag{19}$$

The missing free term in (19) indicates that the initial condition for f^{Δ} is zero, which is a consequence of the assumption that both functions f and f_w^{ϵ} obey the same initial condition. Here we note again the lack of a requirement for a classical interpretation of f: it may be generated by an entirely quantum initial condition.

We are interested in the behavior of $f^{\Delta}(x,p,t)$ for small values ϵ. It can be evaluated by first considering the contribution from the leading term in the series (17) for $\tilde{v}_w$ in (19):

$$\int dp' v_{w,1}^{\epsilon}(x,p-p')f_w^{\epsilon}(x,p',t) = -\epsilon^2\frac{1}{2^2 3!}\frac{d^3v(x)}{dx^3}\frac{d^3}{dp^3}f_w^{\epsilon}(x,p,t). \tag{20}$$

The contribution of this term to the right hand side of (19) is of order ϵ^2 provided that the third derivative of the electric potential and the third momentum derivative $f_w^{\epsilon,3p}$ remain bounded almost everywhere. It is sufficient to request the same for the higher-order terms, to ensure that f^{Δ} is bounded by $M\epsilon^2 t$. It is important to note that this is not just an equivalent way to derive the $E\epsilon$-estimate. While (10) concerns pure state mean values, our result holds for (quasi) distribution functions which provide these mean values in phase space. This gives the opportunity for a generalization towards mixed evolution, where processes of dissipation cause irreversibility.

2.2.5. Towards mixed mode evolution

Electron collisions are described by functions S giving the scattering rates inside a three-dimensional momentum space. It can be shown that the Boltzmann equation has an integral form with a kernel determined by S, whose iterative expansion converges under very general conditions [34]. In particular, it is sufficient that S, being a non-negative function, to be continuous almost everywhere in the momentum domain—the first Brillouin zone. To remain consistent with the x, p phase space utilized in this section, we consider the single-dimensional equivalent of the Boltzmann collision operator $\mathcal{B}f = \int dp' S(p',p)f(p') - \lambda(p)f(p)$ where $S \geq 0$ and $\lambda(p) = \int dp' S(p,p')$. Similar to the three-dimensional counterpart, the corresponding Boltzmann equation $\mathcal{L}f = \mathcal{B}f$, has an integral

form, whose iterative expansion converges. That is, the operator $(\mathcal{I} - \mathcal{L}^{-1}\mathcal{B})^{-1}$ exists, and when applied to a given initial condition the corresponding series converges absolutely for any evolution time t.

When included in our model, this operator appears with a minus sign on the left hand sides of Eqs. (13) (acting on f_w^ϵ) and (16) (acting on f). The result of the subtraction of the two obtained equations is:

$$f^\Delta - \mathcal{L}^{-1}\mathcal{B}f^\Delta = \mathcal{L}^{-1}\tilde{\mathcal{V}}_w^\epsilon f_w^\epsilon. \tag{21}$$

Eq. (21) may be viewed as a Fredholm integral equation of second kind, with a free term given by the expression on the right hand side. It gives rise to the iterative expansion $(I - \mathcal{L}^{-1}\mathcal{B})^{-1}\mathcal{L}^{-1}\tilde{\mathcal{V}}_w^\epsilon f_w^\epsilon$. As this series converges absolutely, we can follow the same logic as in the pure state case to prove the $E\epsilon$-estimate for any particular term, and then to generalize for the whole sum. However, now the function f_w^ϵ, whose derivatives must remain bounded, satisfies a mixed mode evolution equation. An analysis showing that this is not an unrealistic request is given in Appendix B, where convergence and boundedness issues of this case are discussed. In this way the result is generalized to mixed mode transport. It allows to refer to the $E\epsilon$-estimate in Section 3, where interaction with phonons is included in the description.

3. Mixed mode evolution

3.1. Dimensionless wave equation in the presence of phonons

The dynamics of the single electron subject to the action of the electric potential is now generalized to three dimensions, and the interaction with lattice vibrations is taken into account. The description of the system is provided by both electron and phonon coordinates. The Hamiltonian of the system is given by

$$\begin{aligned} H &= H_0 + V + H_p + H_{\text{e-p}} = -\frac{\hbar^2}{2m}\nabla_{\mathbf{R}} + V(\mathbf{R}) + \sum_{\mathbf{Q}} b_{\mathbf{Q}}^\dagger b_{\mathbf{Q}}\hbar\omega_{\mathbf{Q}} \\ &\quad + i\sum_{\mathbf{Q}} \tilde{F}(\mathbf{Q})(b_{\mathbf{Q}}e^{i\mathbf{Q}\hat{\mathbf{R}}} - b_{\mathbf{Q}}^\dagger e^{-i\mathbf{Q}\hat{\mathbf{R}}}) \end{aligned} \tag{22}$$

with the free electron part H_0, the structure potential $V(\mathbf{R})$ the free-phonon Hamiltonian H_p and the electron–phonon interaction $H_{\text{e-p}}$. In the above expressions $b_{\mathbf{Q}}^\dagger$ and $b_{\mathbf{Q}}$ are the creation and annihilation operators for the phonon mode $\mathbf{Q}$, $\hbar\omega_{\mathbf{Q}}$ is the energy of that mode and $\tilde{F}(\mathbf{Q})$ is the electron–phonon coupling element, which depends on the type of phonon scattering analyzed. The position operator $\hat{\mathbf{R}}$ is scaled in the same way as the coordinate R, while the wave vector $\mathbf{Q}$ has the inverse scale:

$$\mathbf{R} = L\mathbf{r}; \qquad \mathbf{Q} = \frac{1}{L}\mathbf{q}; \qquad V(\mathbf{R}) = \eta V_0 v(\mathbf{r}); \qquad \hbar\omega_{\mathbf{Q}} = \alpha V_0 \Omega_{\mathbf{q}}; \qquad \tilde{F}(\mathbf{Q}) = \beta V_0 F(\mathbf{q}). \tag{23}$$

We assumed the same scale for all 3 spatial dimensions, V_0 denotes a given energy scale, so that η, α, β give the relative strength of the different components of the Hamiltonian and are called strength parameters. The time scale is determined again by $T_0 = \sqrt{\frac{m}{V_0}}L$, and the Hamiltonian may be written:

$$\begin{aligned} H &= H_0 + V + H_p + H_{\text{e-p}} = -\frac{\hbar^2}{2mL^2}\nabla_{\mathbf{r}} + \eta V_0 v(\mathbf{r}) + \alpha V_0 \sum_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}}\Omega_{\mathbf{q}} \\ &\quad + i\beta V_0 \sum_{\mathbf{q}} F(\mathbf{q})(b_{\mathbf{q}}e^{i\mathbf{q}\hat{\mathbf{r}}} - b_{\mathbf{q}}^\dagger e^{-i\mathbf{q}\hat{\mathbf{r}}}). \end{aligned} \tag{24}$$

The state of the phonon subsystem is presented by the set $\{n_{\mathbf{q}}\}$, where $n_{\mathbf{q}}$ is the occupation number of the phonons in mode $\mathbf{q}$. Then the representation is given by the vectors $|\{n_{\mathbf{q}}\}, \mathbf{r}\rangle = |\{n_{\mathbf{q}}\}\rangle|\mathbf{r}\rangle$. Since

the whole system is in a pure state, the wave function $\Psi(\{n_{\mathbf{q}}\}, \mathbf{r}) = \langle \{n_{\mathbf{q}}\}, \mathbf{r}|\Psi\rangle$ determines the density matrix:

$$\langle \{n'_{\mathbf{q}}\}, \mathbf{r}'|\rho_t|\{n_{\mathbf{q}}\}, \mathbf{r}\rangle = \Psi^*(\{n_{\mathbf{q}}\}, \mathbf{r})\Psi(\{n'_{\mathbf{q}}\}, \mathbf{r}').$$

The wave function obeys the scaled equation:

$$i\epsilon\frac{\partial \Psi}{\partial t} = \left(-\frac{\epsilon^2}{2}\nabla_{\mathbf{r}} + \eta v(\mathbf{r}) + \alpha\sum_{\mathbf{q}} b^{\dagger}_{\mathbf{q}} b_{\mathbf{q}}\Omega_{\mathbf{q}} + i\beta\sum_{\mathbf{q}} F(\mathbf{q})(b_{\mathbf{q}}e^{i\mathbf{qr}} - b^{\dagger}_{\mathbf{q}}e^{-i\mathbf{qr}})\right)\Psi.$$

3.2. Scaled Wigner models for the electron–phonon system

3.2.1. Generalized Wigner equation

The Wigner function is defined in a way similar to Eq. (12) as:

$$f_w(\mathbf{r}, \mathbf{p}, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}', t) = \frac{1}{(2\pi\epsilon)^3}\int d\mathbf{r}' e^{-i\mathbf{pr}'/\epsilon}\langle \mathbf{r} + \mathbf{r}'/2, \{n_{\mathbf{q}}\}|\hat{\rho}_t|\{n_{\mathbf{q}}\}', \mathbf{r} - \mathbf{r}'/2\rangle.$$

The superscript now becomes $\epsilon, \eta, \alpha, \beta$, but will be omitted in order to simplify the notations. The equation of motion of f_w is then:

$$\frac{\partial f_w(\mathbf{r}, \mathbf{p}, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}', t)}{\partial t} = \frac{1}{i\epsilon}\frac{1}{(2\pi\epsilon)^3} \times \int d\mathbf{r}' e^{-i\mathbf{pr}'/\epsilon}\langle \mathbf{r} + \mathbf{r}'/2, \{n_{\mathbf{q}}\}|\left[H, \hat{\rho}_t\right]_-|\{n_{\mathbf{q}}\}', \mathbf{r} - \mathbf{r}'/2\rangle.$$

Furthermore, we denote the right hand side of the above equation by $WT(H)$. It is evaluated for each component of the Hamiltonian (24). The first two components contribute as:

$$WT(H_0 + v(\mathbf{r})) = -\mathbf{p}\cdot\nabla_{\mathbf{r}} f_w(\mathbf{r}, \mathbf{p}, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}', t) + \eta\int d\mathbf{p}' v_w(\mathbf{r}_1, \mathbf{p} - \mathbf{p}') f_w(\mathbf{r}_1, \mathbf{p}'\{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}', t).$$

The free phonon term is readily evaluated as:

$$WT(H_p) = \frac{\alpha}{i\epsilon}\left(\mathcal{E}(\{n_{\mathbf{q}}\}) - \mathcal{E}(\{n'_{\mathbf{q}}\})\right) f_w(\mathbf{r}, \mathbf{p}, \{n_{\mathbf{q}}\}, \{n_{\mathbf{q}}\}', t),$$

where $\mathcal{E}(\{n_{\mathbf{q}}\}) = \sum_{\mathbf{q}} n_{\mathbf{q}}\Omega_{\mathbf{q}}$. $WT(H_{\text{e-p}})$ gives rise to four terms which are evaluated in one and the same fashion. Beginning with the first one we utilize the decomposition of the identity operator: $\hat{1} = \int d\mathbf{r}''|\mathbf{r}''\rangle\langle\mathbf{r}''|$:

$$\int d\mathbf{r}'\int d\mathbf{r}'' e^{-i\mathbf{pr}'/\epsilon}\left\langle \mathbf{r} + \frac{\mathbf{r}'}{2}, \{n_{\mathbf{q}}\}\right| b_{\mathbf{q}'}e^{i\mathbf{q}'\hat{\mathbf{r}}}|\mathbf{r}''\rangle \times \langle \mathbf{r}''|, \hat{\rho}_t\left|\{n'_{\mathbf{q}}\}, \mathbf{r} - \frac{\mathbf{r}'}{2}\right\rangle = \sqrt{n_{\mathbf{q}'} + 1}e^{i\mathbf{q}'\mathbf{r}} f_w\left(\mathbf{r}, \mathbf{p} - \frac{\epsilon\mathbf{q}'}{2}, \{n_1, \ldots, n_{\mathbf{q}'} + 1, \ldots\}, \{n'_{\mathbf{q}}\}, t\right).$$

We have used the ortho-normality relation $\langle\mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r} - \mathbf{r}')$ and the fact that $b_{\mathbf{q}}$ becomes a creation operator, when operating to the left. The remaining terms are evaluated in a similar way. The resulting scaled generalized Wigner equation is formulated with the help of the short notations $\{n_{\mathbf{q}}\}^{+}_{\mathbf{q}'}$ ($\{n_{\mathbf{q}}\}^{-}_{\mathbf{q}'}$). They describe the states of the phonon subsystem, obtained from $\{n_{\mathbf{q}}\}$ by increasing (decreasing) the number of phonons in the mode $\mathbf{q}'$ by unity.

$$\left(\frac{\partial}{\partial t} + \mathbf{p}\cdot\nabla_{\mathbf{r}}\right) f_w(\mathbf{r}, \mathbf{p}, \{n_{\mathbf{q}}\}, \{n'_{\mathbf{q}}\}, t) = \frac{\alpha}{i\epsilon}\left(\mathcal{E}(\{n_{\mathbf{q}}\}) - \mathcal{E}(\{n'_{\mathbf{q}}\})\right) f_w(\mathbf{r}, \mathbf{p}, \{n_{\mathbf{q}}\}, \{n'_{\mathbf{q}}\}, t)$$

$$
\begin{aligned}
&+\eta\int d\mathbf{p}'v_w(\mathbf{r},\mathbf{p}'-\mathbf{p})f_w(\mathbf{r},\mathbf{p}',\{n_\mathbf{q}\},\{n'_\mathbf{q}\},t)+\frac{\beta}{\epsilon}\\
&\times\sum_{\mathbf{q}'}F(\mathbf{q}')\left\{e^{i\mathbf{q}'\mathbf{r}}\sqrt{n_{\mathbf{q}'}+1}f_w\left(\mathbf{r},\mathbf{p}-\frac{\epsilon\mathbf{q}'}{2},\{n_\mathbf{q}\}^+_{\mathbf{q}'},\{n'_\mathbf{q}\},t\right)\right.\\
&-e^{-i\mathbf{q}'\mathbf{r}}\sqrt{n_{\mathbf{q}'}}f_w\left(\mathbf{r},\mathbf{p}+\frac{\epsilon\mathbf{q}'}{2},\{n_\mathbf{q}\}^-_{\mathbf{q}'},\{n'_\mathbf{q}\},t\right)\\
&-e^{i\mathbf{q}'\mathbf{r}}\sqrt{n'_{\mathbf{q}'}}f_w\left(\mathbf{r},\mathbf{p}+\frac{\epsilon\mathbf{q}'}{2},\{n_{\mathbf{q}'}\},\{n'_\mathbf{q}\}^-_{\mathbf{q}'},t\right)\\
&\left.+e^{-i\mathbf{q}'\mathbf{r}}\sqrt{n'_{\mathbf{q}'}+1}f_w\left(\mathbf{r},\mathbf{p}-\frac{\epsilon\mathbf{q}'}{2},\{n_{\mathbf{q}'}\},\{n'_\mathbf{q}\}^+_{\mathbf{q}'},t\right)\right\}. \qquad (25)
\end{aligned}
$$

The generalized Wigner equation couples an element $f_w(\ldots,\{n\},\{m\},t)$ to four neighboring elements for any phonon mode $\mathbf{q}$. For any such mode, $n_\mathbf{q}$ can be any integer between 0 and infinity and the sum over $\mathbf{q}$ couples all modes. Eq. (25) will be subject to a set of approximations aiming to derive the scaled Wigner–Boltzmann equation. These are the same as in the derivation of the unscaled counterpart, so that only the basic steps will be discussed here. Details can be found in Ref. [25].

3.2.2. Electron Wigner function

We begin with the assumptions which reduce (25) towards a model for the electron Wigner function. The latter is obtained by the trace with respect to the phonon coordinates. Thus the diagonal elements $f_w(\cdot,\{n_\mathbf{q}\},\{n_\mathbf{q}\},\cdot)$ of the generalized WF are of interest. The evolution of an initial state of the system defined at time $t=0$ is considered. The state is assumed diagonal with respect to the phonon coordinates, which corresponds to the evolution process of an initially decoupled electron–phonon system. According to (25), a diagonal element is linked to so called first-off-diagonal elements, which are diagonal in all modes but the current mode $\mathbf{q}'$ of the summation. In this mode the four neighbors of $n_{\mathbf{q}'}, n_{\mathbf{q}'}$ namely $n_{\mathbf{q}'}\pm 1, n_{\mathbf{q}'}$ and $n_{\mathbf{q}'}, n_{\mathbf{q}'}\pm 1$ are concerned. The auxiliary equation for the first first-off-diagonal element $f_w(\cdot,\{n_\mathbf{q}\}^+_{\mathbf{q}'},\{n_\mathbf{q}\},\cdot)$ is obtained again from (25). Accordingly, the first-off-diagonal elements are linked to elements which in general are placed further away from the diagonal ones by increasing or decreasing the phonon number in a second mode, $\mathbf{q}''$, by unity. These are the second-off-diagonal elements. The only exception is provided by two contributions which recover diagonal elements. They are obtained when the running index $\mathbf{q}''$ coincides with $\mathbf{q}'$ in expressions to the type $(\{\{n_\mathbf{q}\}^+_{\mathbf{q}'}\}^-_{\mathbf{q}''},\{n_\mathbf{q}\})$ or $(\{n_\mathbf{q}\}^+_{\mathbf{q}'},\{n_\mathbf{q}\}^+_{\mathbf{q}''})$. Thus the equation is truncated by neglecting all second-off-diagonal elements and keeping only the terms yielding diagonal elements. As a next step, we need to solve the truncated equation, which can be performed explicitly if the Wigner potential term is entirely neglected:

$$
\begin{aligned}
&\left(\frac{\partial}{\partial t}+\left(\mathbf{p}-\frac{\epsilon\mathbf{q}'}{2}\right)\cdot\nabla_\mathbf{r}+i\frac{\alpha}{\epsilon}\Omega_{\mathbf{q}'}\right)f_w\left(\mathbf{r},\mathbf{p}-\frac{\epsilon\mathbf{q}'}{2},\{n_\mathbf{q}\}^+_{\mathbf{q}'},\{n_\mathbf{q}\},t\right)\\
&\quad=\frac{\beta}{\epsilon}F(\mathbf{q}')e^{-i\mathbf{q}'\mathbf{r}}\sqrt{n_{\mathbf{q}'}+1}\left(-f_w(\mathbf{r},\mathbf{p},\{n_\mathbf{q}\},\{n_\mathbf{q}\},t)+f_w(\mathbf{r},\mathbf{p}-\epsilon\mathbf{q}',\{n_\mathbf{q}\}^+_{\mathbf{q}'},\{n_\mathbf{q}\}^+_{\mathbf{q}'},t)\right). \qquad (26)
\end{aligned}
$$

With the help of the trajectory

$$
\begin{aligned}
&\mathbf{p}(t')=\mathbf{p}-\frac{\epsilon\mathbf{q}'}{2}; \qquad (27)\\
&\mathbf{R}(t',\mathbf{q}')=\mathbf{r}-\int_{t'}^{t}d\tau\mathbf{p}(\tau)=\mathbf{r}-\left(\mathbf{p}-\frac{\epsilon\mathbf{q}'}{2}\right)(t-t');
\end{aligned}
$$

initialized at time t by $\mathbf{p}-\frac{\epsilon\mathbf{q}'}{2}$, $\mathbf{r}$, Eq. (26) yields the following integral form.

$$
f_w\left(\mathbf{r},\mathbf{p}-\frac{\epsilon\mathbf{q}'}{2},\{n_\mathbf{q}\}^+_{\mathbf{q}'},\{n_\mathbf{q}\},t\right)=\frac{\beta}{\epsilon}F(\mathbf{q}')\int_0^t dt'e^{-i\frac{\alpha}{\epsilon}\Omega_{\mathbf{q}'}(t-t')}e^{-i\mathbf{q}'\mathbf{R}(t',\mathbf{q}')}\sqrt{n_{\mathbf{q}'}+1}
$$

$$\times \left(f_w(\mathbf{R}(t', \mathbf{q}'), \mathbf{p} - \epsilon\mathbf{q}', \{n_\mathbf{q}\}^+_{\mathbf{q}'}, \{n_\mathbf{q}\}^+_{\mathbf{q}'}, t') \right.$$

$$\left. - f_w(\mathbf{R}(t', \mathbf{q}'), \mathbf{p}, \{n_\mathbf{q}\}, \{n_\mathbf{q}\}, t') \right). \tag{28}$$

Here we have used the fact that the initial condition for first-off-diagonal elements is zero due to the assumption for an initially decoupled system.

The corresponding equation for the second first-off-diagonal element is obtained in the same fashion:

$$f_w\left(\mathbf{r}, \mathbf{p} + \frac{\epsilon\mathbf{q}'}{2}, \{n_\mathbf{q}\}^-_{\mathbf{q}'}, \{n_\mathbf{q}\}, t\right) = \frac{\beta}{\epsilon} F(\mathbf{q}') \int_0^t dt' e^{i\frac{\alpha}{\epsilon}\Omega_{\mathbf{q}'}(t-t')} e^{i\mathbf{q}'\mathbf{R}(t', -\mathbf{q}')} \sqrt{n_{\mathbf{q}'}}$$

$$\times \left(f_w(\mathbf{R}(t', -\mathbf{q}'), \mathbf{p}, \{n_\mathbf{q}\}, \{n_\mathbf{q}\}, t') \right.$$

$$\left. - f_w(\mathbf{R}(t', -\mathbf{q}'), \mathbf{p} + \epsilon\mathbf{q}', \{n_\mathbf{q}\}^-_{\mathbf{q}'}, \{n_\mathbf{q}\}^-_{\mathbf{q}'}, t') \right). \tag{29}$$

The remaining two elements, which complete the diagonal version of (25) give rise to two integral equations which are complex conjugate to the first two. In this way the relevant information is provided by the diagonal equation, and Eqs. (28) and (29), which can be unified into a single equation which contains only diagonal elements of the type:

$$f_w(\{n_\mathbf{q}\}, \{n_\mathbf{q}\}); \qquad f_w(\{n_\mathbf{q}\}^-_{\mathbf{q}'}, \{n_\mathbf{q}\}^-_{\mathbf{q}'}); \qquad f_w(\{n_\mathbf{q}\}^+_{\mathbf{q}'}, \{n_\mathbf{q}\}^+_{\mathbf{q}'}).$$

This gives the opportunity to trace out the phonon coordinates. The assumption that the phonon system is a thermostat for the electrons is used. That is during the evolution the phonons remain in equilibrium $P_{eq}(n_\mathbf{q}) = \frac{e^{-\alpha V_0 \Omega_\mathbf{q} n_\mathbf{q}/kT}}{n(\mathbf{q})+1}$. The trace operation eliminates the phonon degrees of freedom from the equation. Instead, the equilibrium phonon number (Bose distribution):

$$n(\mathbf{q}) = \sum_{n_\mathbf{q}=0}^{\infty} n_\mathbf{q} P_{eq}(n_\mathbf{q}) = \frac{1}{e^{\alpha V_0 \Omega_\mathbf{q}/kT} - 1}$$

appears in the equation. The phonon interaction in the resulting equation still bears the quantum character despite all simplifying assumptions. The main peculiarities are the finite collision time, giving rise to a non-locality in the real space, and the lack of energy conservation.

No approximations are introduced for the coherent part of the transport process: if the phonon interaction is neglected, the common Wigner equation for an electron in an electric potential is recovered.

3.2.3. Scaled Wigner–Boltzmann equation

The energy conserving delta function in the Boltzmann type of interaction is obtained by the following formal limit:

$$\lim_{\epsilon\to 0} \frac{1}{\epsilon} \int_0^\infty d\tau e^{\frac{i}{\epsilon}E\tau} \phi(\tau) = \phi(0) \left\{ \pi\delta(E) + i\mathcal{P}\frac{1}{E} \right\}, \tag{30}$$

involving a delta function and a principal value. We note that the generic function ϕ is evaluated at $\tau = 0$. As applied to the time integrals of the reduced equation, this has the effect of neglecting the duration of the collision processes, while the principal values cancel each-other. This final step gives rise to the scaled Wigner–Boltzmann equation, which with full notations reads:

$$\left(\frac{\partial}{\partial t} + \mathbf{p}\cdot\nabla_\mathbf{r}\right) f_w^{\epsilon,\eta,\alpha,\beta}(\mathbf{r}, \mathbf{p}, t) = \eta \int d\mathbf{p}' v_w^\epsilon(\mathbf{r}, \mathbf{p} - \mathbf{p}') f_w^{\epsilon,\eta,\alpha,\beta}(\mathbf{r}, \mathbf{p}', t)$$

$$+ \int \left(S^{\epsilon,\beta,\alpha}(\mathbf{p}', \mathbf{p}) - \lambda^{\epsilon,\beta,\alpha}(\mathbf{p})\delta(\mathbf{p} - \mathbf{p}') \right) f_w^{\epsilon,\eta,\alpha,\beta}(\mathbf{r}, \mathbf{p}', t) d\mathbf{p}' \tag{31}$$

where $\lambda(\mathbf{p}) = \int S(\mathbf{p}, \mathbf{p}')d\mathbf{p}'$, and the scattering rate S is

$$S^{\epsilon,\beta,\alpha}(\mathbf{p}', \mathbf{p}) = \beta^2 \frac{2\pi}{\epsilon^2} \frac{1}{(2\pi)^3} \left\{ F(\mathbf{q})^2 \delta(\mathbf{p}^2/2 - \mathbf{p}'^2/2 - \alpha\Omega_{\mathbf{q}}) n(\mathbf{q}) + F(\mathbf{q})^2 \delta(\mathbf{p}^2 - \mathbf{p}'^2 + \alpha\Omega_{\mathbf{q}})(n(\mathbf{q}) + 1) \right\}.$$

Here, the delta functions ensure the energy conservation of the processes of phonon absorption and emission, and $\mathbf{q} = (\mathbf{p} - \mathbf{p}')/\epsilon$ arises from the momentum conservation characterizing these processes. For convenience we shorten the equation as follows:

$$\mathcal{L}f_w(\epsilon, \eta, \alpha, \beta) = \eta \mathcal{V}_w^{\epsilon} f_w(\epsilon, \eta, \alpha, \beta) + \beta^2 \mathcal{B}^{\epsilon,\alpha} f_w(\epsilon, \eta, \alpha, \beta). \tag{32}$$

The response of Eq. (31) to an increase of the coupling β with the environment is analyzed in the following.

3.3. Decoherence due to phonons

3.3.1. Scaling theorem

We show that:

Theorem 1. *An increase of the electron–phonon coupling by a factor β' causes a decrease of the strength parameters according to:*

$$\epsilon' = \epsilon/\sqrt{\beta'}, \qquad \eta' = \eta/\beta', \qquad \alpha' = \alpha/\beta'. \tag{33}$$

The evolution problems solved by the Wigner–Boltzmann equation can be divided into classes of equivalence where different physical settings give rise to the same mathematical task.

Proof. It is assumed that initially $\beta = 1$,

$$\mathcal{L}f_w(\epsilon, \eta, \alpha, 1) = \eta \mathcal{V}_w^{\epsilon} f_w(\epsilon, \eta, \alpha, 1) + \mathcal{B}^{\epsilon,\alpha} f_w(\epsilon, \eta, \alpha, 1) \tag{34}$$

after that the electron–phonon coupling is increased from V_0 to $V_0' = V_0\beta'$. The relevant equation has the general form of (32) where the parameter set becomes $\epsilon, \eta, \alpha, \beta'$.

$$\mathcal{L}f_w(\epsilon, \eta, \alpha, \beta') = \eta \mathcal{V}_w^{\epsilon} f_w(\epsilon, \eta, \alpha, \beta') + \beta'^2 \mathcal{B}^{\epsilon,\alpha} f_w(\epsilon, \eta, \alpha, \beta'). \tag{35}$$

This equation can be written in an alternative way provided that V_0' is now used in the scaling relations (23). It holds:

$$\mathcal{L}f_w(\epsilon', \eta', \alpha', 1) = \eta' \mathcal{V}_w^{\epsilon'} f_w(\epsilon', \eta', \alpha', 1) + \mathcal{B}^{\epsilon',\alpha'} f_w(\epsilon', \eta', \alpha', 1). \tag{36}$$

A comparison between (34) and (36) gives the change of the strength parameters:

$$\epsilon' = \frac{\hbar}{L} \frac{1}{\sqrt{m\beta' V_0}}; \qquad \eta' V_0' = \eta V_0 \qquad \alpha' V_0' = \alpha V_0 \tag{37}$$

where the first equality follows from the definition of ϵ, while the other two equalities just state that the rest of the energy factors are kept constant. The Relations (33) follow directly from (37). □

An application of the theorem for analysis of the role of the phonon scattering is given in the next subsection.

Eq. (35) is entirely equivalent to (36) so that the sets $\epsilon', \eta', \alpha', 1$ and $\epsilon, \eta, \alpha, \beta'$ give rise to the same mathematical problem. This shows that from a given choice of the electric potential and length (or time scale), phonon coupling and phonon energies, we may obtain another fully equivalent physical settings by virtue of the scaling theorem. The existence of classes of physically different, but mathematically equivalent problems are illustrated in Section 3.3.3.

3.3.2. Role of the phonon coupling

A comparison between (36) and (34) shows that an increase of the electron–phonon coupling is equivalent to an effective decrease of both, the strength η of the electric potential and the parameter ϵ.

There are two mechanisms, which, in parallel, cause decoherence of the electron system. The first one is directly related to the coupling with the environment. It is expected, and fair, that an increase of the strength of the coupling with the phonon subsystem from unity to $\beta' > 1$ causes a relative decrease of the rest of the parameters in the trio η, α, β. Indeed the classical evolution can be approached either by an increase of the phonon coupling, or by scaling down the Wigner potential. The second mechanism is related to the effect of the strength of scattering on ϵ. According to the $E\epsilon$-estimate, the reduction of this parameter makes the quantum evolution closer to the classical counterpart. In this way the transition towards a classical transport picture is faster than the transition caused by just a linear decrease of the quantum component. It should be admitted that this behavior could be foreseen from the existence of the factor β^2 in (32). However, the scaling theorem gives an insight about the involved physics: For many years the destructive effect of scattering on the quantum behavior has been associated with the vivid picture of electrons which 'carry' the information about the electric potential during the free flight. The reduction of the coherence length is due to the phonon-induced finite lifetime of the electron states [35]. A larger scattering rate gives rise to shorter flights. An alternative estimate of this effect of localization is related to scattering problems, where the dimensions of the wave packet are assumed much larger than the size of the potential a: the latter gives the relevant range of the spatial integral for the Wigner potential [36].

We now suggest a more rigorous and general derivation of the reduction of the coherence length: it is related to the decrease of the quantum correction (19) with the decrease of ϵ, as implied by the $E\epsilon$-estimate. There is a direct way to show this based on the formal correspondence between $\hbar$ and ϵ. Indeed, consider the kernel in the Wigner equation:

$$\begin{aligned}&\frac{1}{i\epsilon 2\pi\epsilon}\int dx'\int dp' e^{-ix'(p-p')/\epsilon} f_w^\epsilon(x,p',t)(v(x+x'/2)-v(x-x'/2))\\&\quad=\frac{d}{dp}\int dx'\left\{\frac{1}{2\pi\epsilon}\int dp' e^{-ix'(p-p')/\epsilon} f_w^\epsilon(x,p',t)\right\}\frac{v(x+x'/2)-v(x-x'/2)}{x'}.\end{aligned}\tag{38}$$

The term in the curly brackets has the form of (30), with a domain of integration from $-\infty$ to ∞. The principal value conveniently falls away, so that the term tends to $f_w(x,p,t)\delta(x')$ with $\epsilon \to 0$. Accordingly, the domain of x' integration shrinks around the origin, which is associated with a reduction of the coherence length. The mathematical aspects of the limit in (38) reuse a well known result for $\hbar \to 0$ [36]. We add to this an insight about the physical factors affecting the limit.

3.3.3. Evolution of entangled states

The existence of classes of physically different, but mathematically equivalent problems will be demonstrated by considering the free evolution of entangled electron states. The latter are initialized by superposition of two Gaussian wave packets $e^{-(X\pm X_0)^2/2\sigma^2}e^{iK_0x}$. Three different sets of physical settings are used, two of them linked by the scaling theorem, while in the third of the parameters is intentionally modified for comparison. It is convenient to switch from momentum to wave vector subspace, where the corresponding initial Wigner function $f_0(X, K_x)$:

$$Ne^{-(K_x-K_0)^2\sigma^2}\left(e^{-\frac{(X-X_0)^2}{\sigma^2}}+e^{-\frac{(X+X_0)^2}{\sigma^2}}+e^{-\frac{X^2}{\sigma^2}}\cos\left((K_x-K_0)2X_0\right)\right)\tag{39}$$

has a well pronounced oscillatory term. Equilibrium is assumed in the other two directions of the wave space, so that $\frac{\hbar^2}{2\pi mkT}e^{-\frac{\hbar^2(K'^2_y+K'^2_z)}{2mkT}}$ multiplies (39) to give $f_w^0(X, \mathbf{K})$. A GaAs semiconductor with a single Γ valley and scattering mechanisms given by elastic acoustic phonons an inelastic polar optical phonons is considered, $X_0 = 70$ nm. A choice of $2\sigma^2 = \hbar^2/(2mkT)$ along with $K_0 = 0$ gives rise to the Maxwell–Boltzmann distribution, which minimizes the effect of the phonons on the change in the shape of the wave vector distribution.

As the electric field is assumed zero the initial Wigner function follows a free evolution, where only phonons interact with the electron state. Phonons cause decoherence by effectively destroying the oscillatory term in the process of evolution. The initially pure state evolves towards an object

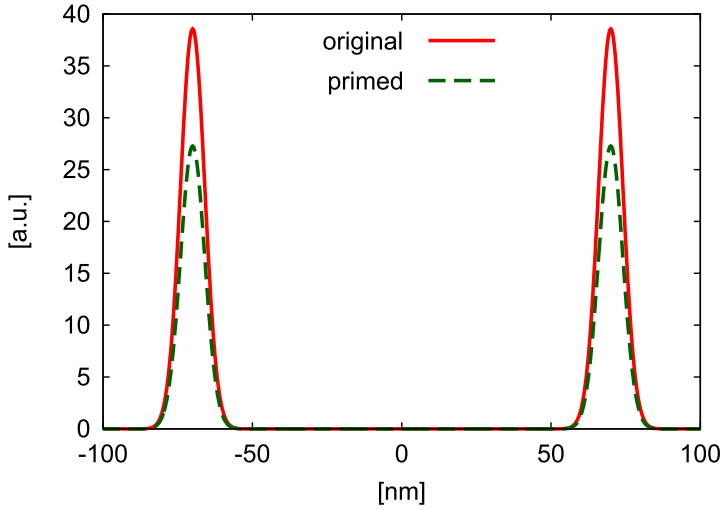

Fig. 1. Initial electron densities of the original and the primed state. A fine structure of positive and negative particles associated with the oscillatory term exists in in the middle between the two peaks. However, their net contribution to the density is zero.

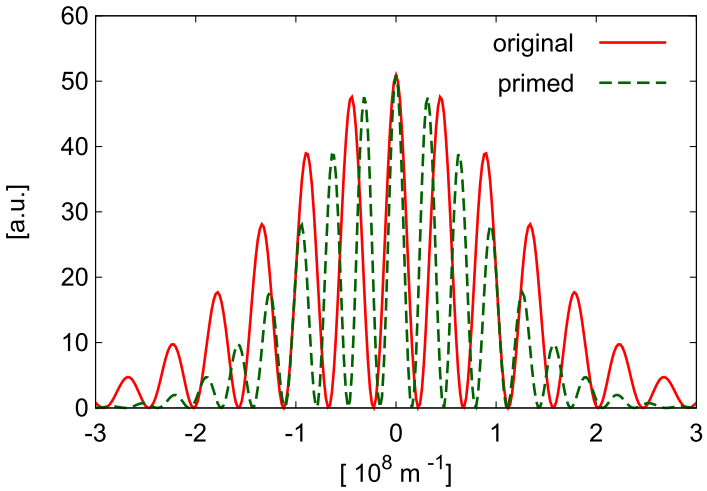

Fig. 2. Initial electron densities of the original and the primed states. The oscillations, caused by the consecutive peaks of positive and negative particles appear at different periods of the wave vector.

having completely different physical meaning: it is a mixed state, determined by the probabilities of the electron to be in one or the other packets related to the two wave functions.

A second entangled state with physical settings is obtained from the original by virtue of the scaling theorem. The parameters of the new system, called primed, are scaled as follows: the spatial set up remains the same, the coupling with the phonons is multiplied by β' : $\tilde{F}' = \beta'\tilde{F}$, the time scale is divided by $\sqrt{\beta'}$: $T_0' = T_0/\sqrt{\beta'}$, the phonon energy is divided by β' : $\alpha' = \alpha/\beta'$, and the wave vector is multiplied by $\sqrt{\beta'}$: $K_o' = K_0\sqrt{\beta'}$, finally β' is chosen to be 2. Thus the two experiments have very different physical characteristics in terms of electron–phonon coupling, phonon energies and initial distributions $f_0(X, K)$ and $f_0(X, \sqrt{\beta'}K)$. However, according to (33) they correspond to one and the same numerical task. The third entangled state violates (33) by an improper scale of the phonon energy $\alpha/\sqrt{\beta'}$. A conventional Monte Carlo method has been utilized to simulate the evolution of the three states. The negative regions of the Wigner function are interpreted as comprised by negative particles, and the particle sign is taken into account when obtaining the physical averages.

Fig. 1 compares the initial densities in arbitrary units. The oscillatory term, which is exactly in the middle between the two peaks is formed by positive and negative particles. These particles compensate each other when taking the averages so that no contribution to the density is visible. Their existence however is well presented in the wave vector distribution, shown in Fig. 2: The oscillations appear at different periods showing the different initial setup. At later times similar oscillations

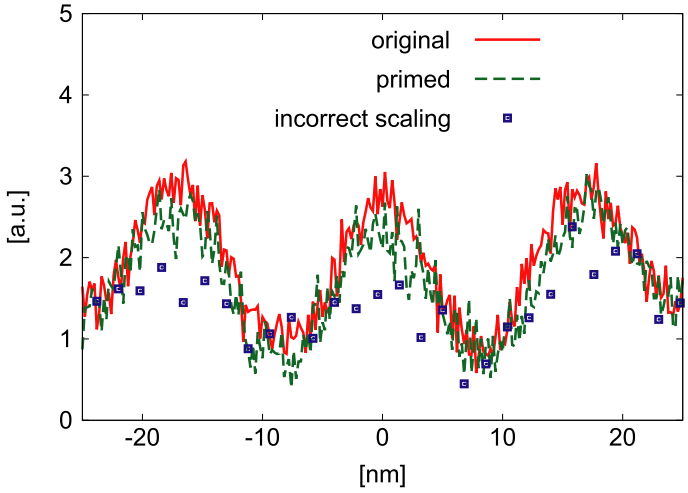

Fig. 3. Electron densities in the central part of the spatial domain. The scaled curves of the original, $T = 210$ fs, and primed experiment $T' = 150$ fs fit well within the stochastic noise, showing that these are completely different stochastic processes, which however give rise to the same distribution of the mean values. An inconsistent scaling of the phonon energy gives rise to a different behavior demonstrated by the different speed of the damping due to the phonons.

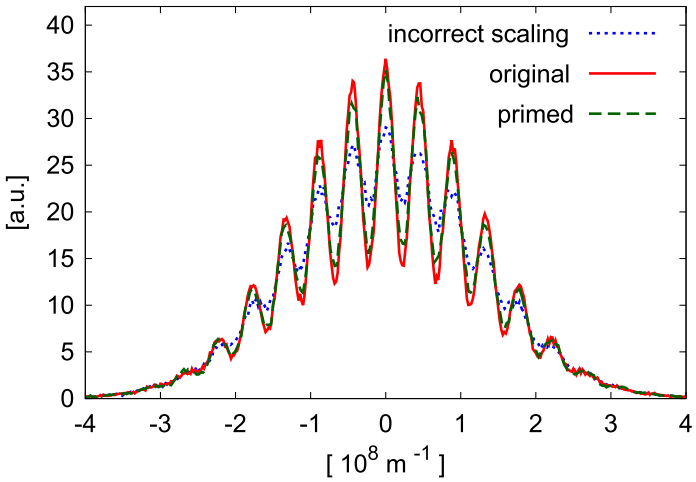

Fig. 4. The scaled according to the scaling theorem momentum densities practically overlap. The oscillations of the incorrectly scaled curve are significantly damped showing how sensitive is the process of decoherence to small changes of the parameter settings.

appear in the density between the two peaks. Such oscillations are characteristics of the coherent evolution. Phonons cause their effective damping with a rate depending on the physical settings. Fig. 3 presents the density in the central part of the spatial domain, and Fig. 4—the momentum distribution. Densities and distributions are adjoined via the scaling theorem, in particular the evolution times are $T = 210$ fs, $T' = 210/\sqrt{2} \simeq 150$ fs for the two systems. The scaled curves overlap, showing that the two experiments correspond to one and the same numerical setup. Indeed, a third experiment which differs by an inconsistent scaling only of the phonon energy shows a completely different behavior. The process of decoherence is very sensitive even to small changes of the parameter settings.

The presented experiments demonstrate the existence of classes of mathematically equivalent physical setups of the Wigner–Boltzmann evolution.

4. Conclusions

The difference between classical and quantum expectation values of given physical observables is estimated with the help of the parameter ϵ, determined by the physical scales involved in the system.

The estimation is based on the scaled Schrödinger equation, which provides a relevant formalism for the pure state evolution of the system. The result is then reformulated in terms of classical and Wigner phase space distribution functions, and generalized for mixed mode evolution caused by a single-dimensional scattering term. The problem is then augmented to three dimensions to explore the interplay of the physical scales in determining the transport regime. Dimensionless parameters corresponding to the relative strength of the energy scales of the device potential, the phonon energy and the electron–phonon coupling are used to derive the dimensionless Wigner–Boltzmann equation, and to trace the appearance of these parameters in the model. The scaling theorem derives the dependencies of these parameters on the phonon coupling. The theorem gives an insight on the mechanisms causing decoherence and the process of electron localization. Another application demonstrates the existence of classes of mathematically equivalent physical setups of the Wigner–Boltzmann evolution.

Acknowledgments

This work has been partially supported by: the Austrian Science Fund (FWF) P21685-N22, the French "Agence Nationale de la Recherche" under project MODERN (ANR-05-NANO-002), the USA NSF Grant ECCS 0901251 (PD P. Werbos) and the Bulgarian Science Fund under grant DTK 02/44.

Appendix A. Natural parameter values

Here, we consider a choice of scales for the physical quantities, which is especially convenient from a heuristic point of view. The results are particularly related to semiconductor carriers, as the Wigner picture becomes a promising approach to transport in nanoelectronic devices. Within the same notations as used for the scale factors L, V_0, T_0 of distance, energy, and time, we introduce the values $T_0 = \frac{\hbar}{V_0}$, $L = \sqrt{\frac{\hbar^2}{mV_0}}$ which define the natural length and time scale. For example, the latter arises when ϵ is set to unity, and gives the corresponding length scale for which the quantization energy is roughly equal to the potential energy peak. The quantity T_0 may be interpreted as the coherence time necessary to see the quantum effects. Let us consider an example. If the maximum potential is e.g. 0.1 eV, then the natural time scale is 6.6 femtoseconds, and the natural length scale is 3.4 nanometers for *GaAs*. These values are on the scale of a few time steps and grid spacings which are used in most simulations. This corresponds to the choice $\epsilon = 1$, which makes (3) free of any parameters. But, the time is quite small. A more normal value for the typical scattering time in GaAs is about 0.2 ps, which would set the natural potential value to 3.3 meV. This gives a much smaller role to the scattering, since most potentials will be larger than this value. Correspondingly, the natural length scale now becomes about 18.6 nm. Such sets of natural values give an opportunity to examine the manner in which quantization enters the problem. Now, instead of starting from the consistency considerations used to obtain (15), we start from the commutator relationship $[\hat{X}, \hat{P}]_- = i\hbar$.

This will be used to introduce another parameter, η, which is a normalization of the momentum itself: $\hat{P} = -i\hbar\frac{\partial}{\partial X} = -i\frac{\hbar}{L}\frac{\partial}{\partial x} = \eta\hat{p}$. Now, the commutator becomes $[\hat{x}, \hat{p}]_- = i\eta$, $\eta = \frac{\hbar}{L} = \sqrt{mV_0}$. This result for η is entirely in accordance with the expression for P_0 after Eq. (15). Indeed, if the definition of the natural time is applied, it follows that $P_0 = \eta$. The meaning of η is clear. If L is a natural length for quantization, then η is roughly the uncertainty in momentum that arises from this length.

In the natural scheme the normalization of the momentum is set by the momentum value which corresponds to the reference potential height. For our values above, and *GaAs*, this constant is 1.4×10^{25} kg m/s.

The importance of this approach is that any time η appears (or any time η is not negligible in comparison to this value), it is a signal that quantization is important. We also note that the exponentials of the Weyl transforms are now free of any parameters, as $\frac{XP}{\hbar} \to xp$ which is consistent with the choice $\eta(T_0, V_0) = 1$. From the last expression it follows that we have basically one free parameter and this is the reference potential height.

Appendix B. Convergence and boundedness

We discuss convergence and boundedness issues of a mixed mode evolution described by an equation, which may be considered as a single-dimensional equivalent of the Wigner–Boltzmann equation. The existence of the mixed mode solution follows from the separate convergence of the Boltzmann and pure state iterative expansions. In contrast to the Boltzmann case, the absolute convergence of the integral form of (13) is guaranteed for times less than a time T_0 related to the upper bound of the absolute value of the Wigner potential. The existence of solution for given time T can be then shown by using the Markovian character of the evolution, where the evolved state is considered as an initial condition for the next T_0-interval of the evolution. We consider (13) for $t < T_0$ so that $(\mathcal{I}-\mathcal{L}_w^{-1}\mathcal{V}_w^{\epsilon})^{-1}$ gives rise to an absolutely convergent series when applied to a given bounded function f_0. As the same holds for the Boltzmann counterpart, there follows the existence of the solution for the equation:

$$\mathcal{L}_w f_w^{\epsilon} = (\mathcal{V}_w^{\epsilon} + \mathcal{B}) f_w^{\epsilon}. \tag{B.1}$$

Finally, we assume that S and f_0 have bounded derivatives to all orders with respect to p. The equation for the first derivative $f_w^{\epsilon,p}$ of f_w^{ϵ} is obtained by differentiating (B.1) with respect to p:

$$\begin{aligned}\frac{\partial f_w^{\epsilon,p}(x,p,t)}{\partial t} + p\frac{\partial f_w^{\epsilon,p}(x,p,t)}{\partial x} &= \int dp' v_w^{\epsilon}(x,p') \times f_w^{\epsilon,p}(x,p-p',t) \\ &\quad + \Gamma(x,p,t) - \lambda(p) f_w^{\epsilon,p}(x,p,t)\end{aligned} \tag{B.2}$$

with

$$\Gamma(x,p,t) = \int dp' \frac{\partial S}{\partial p}(p',p) f_w^{\epsilon}(x,p',t) - \frac{\partial \lambda(p)}{\partial p} f_w^{\epsilon}(x,p,t) - \frac{\partial f_w^{\epsilon}(x,p,t)}{\partial x}.$$

Eq. (B.2) has the following integral form:

$$\begin{aligned}f_w^{\epsilon,p}(x,p,t) &= \int_0^t dt' e^{-\lambda(p)(t-t')} \int dp' v_w^{\epsilon}(X(t'),p') f_w^{\epsilon,p}(X(t'),p-p',t') \\ &\quad + \int_0^t dt' e^{-\lambda(p)(t-t')} \Gamma(X(t'),p,t') + e^{-\lambda(p)t} f_0^p(X(0),p)\end{aligned} \tag{B.3}$$

which may be proved by a direct differentiation. The trajectory $X(t') = x - \frac{p}{m}(t-t')$ is initialized by the arguments of the function $f_w^{\epsilon,p}$ on the left, while f_0^p is the first p derivative of the initial condition. In this way $f_w^{\epsilon,p}$ is a solution of a Fredholm integral equation of the second kind with a free term given by the second row in (B.3). The solution presented by the resolvent series is a sum of terms given by the consecutive applications of the kernel on the free term. The exponential damping term in the kernel only improves the convergence as compared with the Wigner counterpart. According to our assumptions the free term is bounded so that the same may be concluded for the first derivative $f_w^{\epsilon,p}$. The equation for the second derivative is obtained by differentiating (B.2). The obtained equation allows the same analysis and the procedure may be continued for higher order derivatives.

The auxiliary function S conveniently allows to carry out the above analysis in the single-dimensional phase space. The existence of derivatives of S may be weakened to almost everywhere since it always appears under a p integration. Moreover, the realistic three dimensional scattering functions S contain energy and momentum conserving delta functions which greatly reduce the relevant momentum space to a subdomain of the Brillouin zone, and prefactors which are usually rational or with 'good' properties as functions of the momenta. Thus the requirement for bounded derivatives is not unrealistic. Of central importance remains the need of all derivatives of the initial condition (and the same for the electric potential).

References

[1] H. Weyl, Zeitschrift für Physik 46 (1927) 1–46.
[2] E. Wigner, Physical Review 40 (1932) 749–759.
[3] N.C. Dias, J.N. Prata, Annals of Physics 313 (2004) 110–146.
[4] E.A. Remler, Annals of Physics 95 (1975) 455–495.
[5] W.H. Zurek, Reviews of Modern Physics 75 (3) (2003) 715–775.
[6] M. Schlosshauer, Reviews of Modern Physics 76 (2005) 1267–1305.
[7] J.P. Paz, W.H. Zurek, Physical Review Letters 82 (1999) 5181–5184.
[8] J. Eisert, Physical Review B 92 (2004) 210401.
[9] D.K. Ferry, Akis, J.P. Bird, Physical Review Letters 93 (2004) 026803.
[10] F. Buscemi, P. Bordone, A. Bertoni, Physica Status Solidi (c) 5 (2008) 52–55.
[11] M. Hofheinz, H. Wang, M. Ansmann, R.C. Bialczak, E. Lucero, M. Neeley, A.D. O'Connell, D. Sank, J. Wenner, J. Martinis, A.N. Cleland, Physical Review B 92 (2004) 210401.
[12] I. Knezevic, Physical Review B 77 (2008) 125301.
[13] M. Nedjalkov, H. Kosina, S. Selberherr, C. Ringhofer, D. Ferry, Physical Review B 70 (11) (2004) 115319–115335.
[14] D. Querlioz, P. Dollfus, The Wigner Monte Carlo Method for Nanoelectronic Devices—A Particle Description of Quantum Transport and Decoherence, ISTE-Wiley, 2010.
[15] D. Querlioz, J. Saint-Martin, A. Bournel, P. Dollfus, Physical Review B 78 (2008) 165306.
[16] J. Lin, L.C. Chiu, Journal of Applied Physics 57 (1985) 1373.
[17] I. Levinson, Soviet Physics JETP 30 (2) (1970) 362–367.
[18] W. Frensley, Physical Review B 36 (3) (1987) 1570–1580.
[19] R.K. Mains, G.I. Haddad, Journal of Applied Physics 64 (1988) 5041–5044.
[20] L. Shifren, C. Ringhofer, D. Ferry, IEEE Transactions on Electron Devices 50 (3) (2003) 769–773.
[21] W. Frensley, Reviews of Modern Physics 62 (3) (1990) 745–789.
[22] N.C. Kluksdahl, A.M. Kriman, D.K. Ferry, C. Ringhofer, Physical Review B 39 (1989) 7720–7734.
[23] D. Querlioz, H.N. Nguyen, J. Saint-Martin, A. Bournel, S. Galdin-Retailleau, P. Dollfus, Journal of Computational Electronics 8 (2009) 324–335.
[24] M. Nedjalkov, Proceedings of the International School of Physics 'Enrico Fermi', in: A.P.A. D'Amico, G. Balestrino (Eds.), From Nanostructures to Nanosensing Applications, vol. 160, IOS Press, Amsterdam, 2005, pp. 55–103.
[25] M. Nedjalkov, D. Querlioz, P. Dollfus, H. Kosina, in: D. Vasileska, S. Goodnick (Eds.), Nano-Electronic Devices: Semiclassical and Quantum Transport Modeling, Springer-Verlag, ISBN: 978-1-4419-8839-3, 2011, pp. 289–358. invited.
[26] A. Bouzouina, D. Robert, Duke Mathematical Journal 111 (2002) 223–252.
[27] J. Bolte, R. Glaser, Communications in Mathematical Physics 247 (2004) 391–419.
[28] C. Lasser, S. Röblitz, SIAM Journal on Scientific Computing 32 (2010) 1465–1483.
[29] D. Bambusi, S. Graffi, T. Paul, Asymptotic Analysis 21 (1999) 149–160.
[30] C. Jacoboni, Theory of Electron Transport in Semiconductors, Springer, 2010.
[31] O. Baumgartner, P. Schwaha, M. Karner, M. Nedjalkov, S. Selberherr, Coupling of non-equilibrium Green's function and Wigner function approaches, in: Proc. Simulation of Semiconductor Processes and Devices, Hakone, Japan, ISBN: 978-1-4244-1753-7, 2008, pp. 931–934.
[32] P. Schwaha, O. Baumgartner, R. Heinzl, M. Nedjalkov, S. Selberherr, I. Dimov, 13th International Workshop on Computational Electronics, IWCE-13, IEEE, Beijing, China, ISBN: 978-1-4244-3927-0, 2009, pp. 177–180.
[33] A. Polkovnikov, Annals of Physics 325 (2010) 1790–1852.
[34] M. Nedjalkov, D. Vasileska, I. Dimov, G. Arsov, Monte Carlo Methods and Applications 13 (4) (2007) 299–331.
[35] J. Barker, D. Ferry, Solid State Electronics 23 (1980) 519–549.
[36] P. Carruthers, F. Zachariasen, Reviews of Modern Physics 55 (1) (1983) 245–285.