

On quantum extensions to classical Spherical Harmonics Expansion / Fokker-Planck models

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Abstract

By following a strategy introduced in previous works, quantum extensions of the classical electron-phonon scattering operator are deduced from first principles. These quantum collision operators satisfy a quantum H-theorem and relax towards quantum equilibria. Then, under an assumption of dominant elastic interactions, a hierarchy of quantum Spherical Harmonic Expansion (SHE) models is derived by a diffusive approximation of collisional Wigner equations. These models are proven entropic and their expansions into powers of the reduced Planck constant \hbar are calculated, leading to \hbar^2 corrections for the classical SHE model.

1 Introduction

The transport of charged particles in electronic devices is generally described by kinetic models such as Boltzmann-like equations or macroscopic models of hydrodynamic or diffusion type. Due to the ongoing miniaturization of these devices, reaching the nanometric scale, the reliability of these classical models becomes doubtful as quantum effects become important. Since, at an intermediate scale, collision phenomena remain significant, one of the most challenging areas of investigation in semiconductor modelling deals with the setting-up of quantum transport models which take into account scattering effects. Though many works are concerned with the numerical simulation of ballistic quantum transport models for semiconductors (see *e.g.* [27, 38, 45, 26, 16, 47]), a quantum theory of collisions is still under development (among other works on the quantum theory of scattering, see *e.g.* [3, 13, 25, 39, 48] and, more recently, [4, 6, 28]). Furthermore, several attempts were made to adapt existing classical macroscopic models to quantum mechanics [1, 2, 31, 32, 33, 34] but, generally, the link between the so-obtained models and a microscopic quantum description of the particle transport is to a large extent phenomenological.

Recently, a strategy for deriving quantum macroscopic models was introduced in [22, 23]. It relies on the notion of a quantum local equilibrium (called “quantum Maxwellian”), defined through a Gibbs principle as the minimizer of the quantum entropy under local moment constraints. This approach enabled to write prototypes of collision operators which decrease the quantum entropy and relax towards the quantum local equilibria. By introducing such collision operators in the Wigner equation and by performing formally a hydrodynamic (resp. diffusive) limit, quantum hydrodynamic (resp. quantum diffusive) models were derived in [22] and [20] (these two papers are reviewed in [21]). As a by-product of the method, these quantum macroscopic models display some interesting physical properties, such as the preservation

of the positivity of the density or an entropy dissipation. The numerical resolution of the simplest of these models, the quantum drift-diffusion model, is investigated in [29, 30].

The small size of current semiconductor devices raises another problem. In some regimes, the relevant time and length scales are too small for the cloud of electrons to reach a thermodynamical equilibrium. Therefore, an accurate description of these devices cannot be achieved by models which, like drift-diffusion or hydrodynamic models, rely on the assumption that the system has been driven to an equilibrium with a given profile (of Maxwellian or of Fermi-Dirac type). Intermediate models have been recently introduced, in a classical setting, to fill the gap between precise but numerically expensive models (kinetic models for instance) and numerically affordable but less accurate models such as drift-diffusion models: among others are the Spherical Harmonics Expansion (SHE) models (see [7, 15] for a mathematical description and references). These models are diffusion models in the position-energy space. They have been applied to semiconductor physics ([35, 11, 12, 8, 9]), neutronics ([36]), gas discharge ([49]) and plasma physics ([24]). Numerical computations have established the relevance of the classical SHE models ([18, 10]). These models are also referred to as Fokker-Planck models. They consist of a mass balance equation (the continuity equation) for the energy distribution function, and of a constitutive law for the current of particles of given energy. The former governs the transport of the density and the latter describes the effects of the diffusion due to the particle scattering.

The goal of this paper is twofold. On the one hand, following the strategy, described above, which leads to deriving quantum versions of the hydrodynamic (HD), energy-transport (ET) and drift-diffusion (DD) models, we propose quantum SHE models. These models are expected to be better adapted than classical SHE

models to situations where quantum phenomena are predominant. Moreover, as in the classical case where SHE models appear as intermediate models between kinetic and macroscopic equations, quantum SHE models fit systems far from Maxwellian-like equilibria better than quantum HD, ET and DD models.

The derivation of quantum SHE models by a diffusion approximation procedure makes the introduction of quantum collision operators at the kinetic level necessary: this constitutes the second goal of this work. A quantum collision operator is built following ideas first introduced in [22, 23, 20] and generalizing the classical electron-phonon scattering operator [41]. Then, in the regime of dominant elastic scattering, several other operators are proposed. All these operators are consistent with the elementary properties which are sought to describe collisions with phonons (conservations, equilibrium states, quantum entropy dissipation).

The paper is organized as follows. Section 2 recalls some well-known results about the derivation of classical SHE models and emphasizes the importance of the entropy dissipation of the collision operator to obtain an entropic structure for the macroscopic model. Classical features of the linearized electron-phonon collision operator are also recalled. Section 3 is a first step towards the derivation of a quantum SHE model: we consider the Wigner equation equipped with a classical collision operator and perform the derivation in this setting, which leads to the Quasi-Quantum SHE model. This model does not account for quantum diffusion. Quantum collision operators are introduced in Section 4 following a heuristic analogy: these operators must fulfill properties analogue to those satisfied by the classical operators given in Section 2. For this sake, a quantum entropy is given and quantum thermodynamical equilibria are defined as minimizers of this entropy, allowing the introduction of quantum relaxation operators. Then the derivation of a fully quantum SHE model can be performed and this is achieved in Section 5.

The Quantum SHE and Quasi-Quantum SHE models involve pseudo-differential operators and display a non-local character. In order to obtain models easier to handle, a formal expansion of these equations with respect to the reduced Planck constant \hbar are given in Sections 3 and 5. As it was done in [20] for the quantum energy-transport and the quantum drift-diffusion models, by keeping only the terms up to second order in \hbar in this expansion, we derive quantum correction terms for the classical SHE model.

2 Classical modelling of Electron-Phonon Scattering in semiconductor devices: a short review

In this section, we review some well-known features concerning electron-phonon scattering in classical kinetic models. Indeed, having this review in mind will help understand our methodology for establishing quantum collision operators and deriving various quantum SHE models.

2.1 The Boltzmann equation

The evolution of electrons in semiconductor devices can be described at a microscopic level through classical kinetic equations of Boltzmann type as long as quantum effects are neglected. To that purpose, one introduces the distribution function $f(t, x, p)$ of the electrons. Then f is given as the solution of the initial value problem

$$\begin{cases} \partial_t f + p \cdot \nabla_x f - \nabla_x V \cdot \nabla_p f = \mathcal{C}(f), & x \in \mathbb{R}^3, p \in \mathbb{R}^3, t > 0 \\ f(0, x, p) = f_I(x, p) \end{cases} \quad (2.1)$$

where $V = V(x)$ is a given potential and f_I an initial condition. The collision operator \mathcal{C} models the interactions of the electrons with the medium. All the quantities

that will be considered in the sequel are dimensionless. The equation is adimensional and we set the temperature equal to 1 and the electron mass and elementary charge equal to 1 and -1 respectively. We will note

$$L = p \cdot \nabla_x - \nabla_x V \cdot \nabla_p$$

the classical transport (Liouville) operator. The classical relative entropy usually associated to this kind of equation is

$$H_C(f) = \int_{\mathbb{R}^6} f \left(\ln f - 1 + \frac{|p|^2}{2} + V(x) \right) dx dp = \int_{\mathbb{R}^6} f \left(\ln \frac{f}{\mathcal{M}} - 1 \right) dx dp$$

where the global Maxwellian \mathcal{M} is defined by

$$\mathcal{M}(x, p) = \exp \left(-\frac{|p|^2}{2} - V(x) \right). \quad (2.2)$$

When the context is clear, we will note as well $\mathcal{M}(x, \varepsilon) = \exp(-\varepsilon - V(x))$, where ε denotes the energy variable ($\varepsilon \geq 0$). The following lemma is a classical result on H_C . Its proof is straightforward.

Lemma 2.1 *Let \mathcal{C} in (2.1) be such that, for any positive measurable function g , this inequality holds:*

$$- \int \mathcal{C}(g) \ln \left(\frac{g}{\mathcal{M}} \right) dx dp \geq 0. \quad (2.3)$$

Then, if f is a positive solution of Eq. (2.1), the associated entropy satisfies:

$$\frac{dH_C(f)}{dt} \leq 0. \quad (2.4)$$

According to this lemma, the study of the entropic structure of equations of type (2.1) reduces to proving an inequality on the collision operator \mathcal{C} . In this section, several collision operators are introduced in order to model the scattering of electrons in semiconductors. The classical electron-phonon collision operator is introduced

and some of its properties are recalled. The limit of a vanishing phonon energy is performed and yields an elastic collision operator. Then, the derivation of a classical SHE model is set out (following [7, 15]) and its entropic structure is emphasized.

Before achieving these tasks, we introduce the spherical coordinates in momentum space: $\omega = p/|p| \in \mathbb{S}^2$, $\varepsilon = |p|^2/2 > 0$, where \mathbb{S}^2 denotes the unit sphere in \mathbb{R}^3 . For any function f , we note equally $f(p) = f(\varepsilon, \omega)$ and, when the context is unambiguous, $f = f(p)$ and $f' = f(p')$. The following formula holds for any integrable function f

$$\int_{\mathbb{R}^3} f(p) dp = \int_{(0, \infty) \times \mathbb{S}^2} f(\varepsilon, \omega) \sqrt{2\varepsilon} d\varepsilon d\omega$$

and we define

$$\int_{\mathbb{R}^3} f(p') \delta(|p'|^2/2 - \varepsilon) dp' = \int_{(0, \infty) \times \mathbb{S}^2} f(\varepsilon', \omega') \delta(\varepsilon' - \varepsilon) \sqrt{2\varepsilon'} d\varepsilon' d\omega' := \sqrt{2\varepsilon} \int_{\mathbb{S}^2} f(\varepsilon, \omega') d\omega'.$$

Let $L^2_{x,p} = L^2(\mathbb{R}^6)$ denote the space of square integrable functions on the phase space \mathbb{R}^6 . The closed subspace of energy dependent functions will be of considerable interest in the remainder of the paper and is denoted by

$$\mathcal{E} = \{f \in L^2_{x,p} : f(x, p) = f(x, |p|) \text{ a.e.}\}$$

and the space orthogonal to \mathcal{E} in $L^2_{x,p}$ is denoted by \mathcal{E}^\perp . The projectors on \mathcal{E} and on \mathcal{E}^\perp are respectively denoted by \mathcal{P} and \mathcal{P}^\perp and, for any ϕ in $L^2_{x,p}$, they are given by

$$\mathcal{P}(\phi)(\varepsilon) = \frac{1}{N(\varepsilon)} \int_{\mathbb{R}^3} \phi(\varepsilon', \omega') \delta(\varepsilon' - \varepsilon) dp', \quad \mathcal{P}^\perp \phi = (\text{Id} - \mathcal{P})\phi$$

where Id denotes the identity operator on $L^2_{x,p}$ and $N(\varepsilon)$, the density of state, is defined by

$$N(\varepsilon) = \int_{\mathbb{R}^3} \delta(|p'|^2/2 - \varepsilon) dp' = 4\pi\sqrt{2\varepsilon},$$

so that the projector \mathcal{P} can be written equivalently as

$$\mathcal{P}(\phi)(\varepsilon) = \frac{1}{4\pi} \int_{\mathbb{S}^2} \phi(\varepsilon, \omega') d\omega'.$$

Note that, for any f and ϕ , $\mathcal{P}(\phi f) = \phi \mathcal{P}(f)$ and $\mathcal{P}^\perp \phi = 0$ as soon as ϕ is a function of the energy ε only. Moreover, \mathcal{E}^\perp is spanned by functions of null angular average.

2.2 The Classical Electron-Phonon collision operator

We now focus on the expression of the collisions operator $\mathcal{C}(f)$. In semiconductors, electrons undergo mainly three types of collisions against ionized impurities, acoustic phonons and optical phonons [50]. At large enough energies, optical phonon collisions are dominant and we shall discard the other types of collisions.

Classically (see [44] for instance), in a low density case, the electron-optical phonon collision operator is linear and can be written, after an appropriate scaling, according to

$$\begin{aligned} \mathcal{C}_{e\varphi}(f)(p) = & \int \Sigma(p, p') \{ [(N_0 + 1)\delta(\varepsilon - \varepsilon' + \beta) + N_0\delta(\varepsilon - \varepsilon - \beta)] f(p') \\ & - [(N_0 + 1)\delta(\varepsilon' - \varepsilon + \beta) + N_0\delta(\varepsilon' - \varepsilon - \beta)] f(p) \} dp' \end{aligned}$$

with β the scaled phonon energy (which is a constant), $\Sigma(p, p')$ a symmetric function of the form

$$\Sigma(p, p') = C_{\text{opt}}\beta \begin{cases} \frac{1}{|p-p'|^2} & \text{(polar interactions)} \\ 1 & \text{(non polar interactions)} \end{cases} \quad (2.5)$$

where C_{opt} is an appropriate constant. The phonon occupation number N_0 for a lattice temperature $T = 1$ is given by the Bose-Einstein statistics as:

$$N_0 = \frac{1}{e^\beta - 1}. \quad (2.6)$$

The collision operator can also be written

$$\mathcal{C}_{e\varphi}(f) = \int \mathcal{S}(p, p') [\delta(\varepsilon' - \varepsilon - \beta) + \delta(\varepsilon' - \varepsilon + \beta)] \left(\frac{f(p')}{M(\varepsilon')} - \frac{f(p)}{M(\varepsilon)} \right) dp' \quad (2.7)$$

with $M = M(\varepsilon) = \exp(-\varepsilon)$ the Maxwellian and

$$\mathcal{S}(p, p') = \Sigma(p, p') N_0 e^{-(\varepsilon+\varepsilon')/2} e^{\beta/2},$$

which is a symmetric function. The following result can be found in [41]:

Proposition 2.2 *The collision operator $\mathcal{C}_{e\varphi}$ defined by (2.7) satisfies the following properties:*

(i) *Mass conservation: $\int \mathcal{C}_{e\varphi}(f)dp = 0$ for any measurable function f .*

(ii) *Equilibrium states: for any measurable function $f(x, p)$, we have $\mathcal{C}_{e\varphi}(f) = 0$ if and only if*

$$f(x, p) = M(|p|^2/2)F(x, |p|^2/2)$$

where F is such that $F(x, \varepsilon + \beta) = F(x, \varepsilon)$.

(iii) *Entropy dissipation: $-\int \mathcal{C}_{e\varphi}(f) \ln(f/\mathcal{M})dp \geq 0$ for any positive integrable function f .*

Typically, the electron energy in a semiconductor device is of the same order of magnitude as the applied bias, *i.e.* of the order of 1 Volt. This is very large compared with the typical optical phonon energy, which is of the order of 10^{-2} Volts. Therefore, the scaled parameter $\beta \approx 10^{-2}$ is very small and it is meaningful to consider the elastic limit $\beta \rightarrow 0$ of the electron-phonon collision operator.

The following operator \mathcal{C}_{el} can be obtained as the limit of $\mathcal{C}_{e\varphi}$ as $\beta \rightarrow 0$:

$$\mathcal{C}_{el}(f)(p) = N(|p|^2/2) \left\{ \mathcal{P} \left(\tilde{\mathcal{S}}(p, \cdot) f(\cdot) \right) - \mathcal{P} \left(\tilde{\mathcal{S}}(p, \cdot) \right) f(p) \right\} \quad (2.8)$$

where

$$\tilde{\mathcal{S}}(p, p') = 2 C_{\text{opt}} \begin{cases} \frac{1}{|p-p'|^2} & \text{(polar interactions),} \\ 1 & \text{(non polar interactions).} \end{cases} \quad (2.9)$$

From now on, we drop the tildas. It is straightforward to prove that

Proposition 2.3 *The collision operator \mathcal{C}_{el} defined by (2.8) satisfies the following properties:*

(i) *Mass conservation: $\int \mathcal{C}_{el}(f)dp = 0$ for any measurable function f .*

(ii) *Equilibrium states: for any function f in $L^2_{x,p}$, we have $\mathcal{C}_{el}(f) = 0$ if and only if*

$$f(x, p) = F(x, |p|^2/2)$$

where F lies in \mathcal{E} .

(iii) *Entropy dissipation*: $-\int \mathcal{C}_{el}(f) \ln(f/\mathcal{M}) dp \geq 0$ for any positive integrable function f .

2.3 Derivation of the Classical SHE model (CSHE)

Classical SHE models (CSHE) (also referred to as Fokker-Planck models) are obtained as asymptotic limits of the Boltzmann equation under the assumption of dominant elastic scattering, *i.e.* when the collision operator (of the type (2.8)) is supposed to be large, say of order $1/\alpha$ where α is a measure of the collision mean-free path in scaled units. We also need to observe the system over large periods of time, *i.e.* we must rescale the time variable $t \rightarrow t/\alpha$ in order to capture the significant dynamics, which is of diffusion type. In this new set of units, the classical Boltzmann equation becomes:

$$\alpha \partial_t f^\alpha + (p \cdot \nabla_x - \nabla_x V \cdot \nabla_p) f^\alpha = \frac{1}{\alpha} \mathcal{C}_{el}(f). \quad (2.10)$$

To ensure boundedness and positivity for the collision operator, we assume that

Assumption 2.4 *There exist two positive constants K, K' such that $K < \mathcal{S} < K'$.*

Under this assumption, operator \mathcal{C}_{el} is an isomorphism from \mathcal{E}^\perp onto \mathcal{E}^\perp (see [7] for instance). Then, Equation (2.10) has solutions according to the Hille-Yosida theorem:

Lemma 2.5 *Under regularity assumptions on the potential V and Assumption 2.4, Eq. (2.10) with initial datum f_I in $\mathcal{D}(L) := \{f \in L^2_{x,p} : Lf \in L^2_{x,p}\}$ has a unique solution f^α in $C^1([0, T], L^2_{x,p}) \cap C^0([0, T], \mathcal{D}(L))$.*

We do not enter into details regarding sufficient assumptions on V since the differential operator $\nabla_x V \cdot \nabla_p$ will not be used in this paper, but, instead, an L^2 bounded pseudo-differential operator. The (possibly not optimal) regularity required for V in the quantum case is stated in Assumption 3.2 below.

Proposition 2.6 summarizes some results on the derivation of the CSHE model (see [7] and [15] for this proposition as well as for precise regularity requirements on the potential V):

Proposition 2.6 *Assumption 2.4 is made and V is supposed regular enough.*

We consider Eq. (2.10) with initial datum f_I^α such that the sequence (f_I^α) converges in $L^2_{x,p}$ to an element F_{in} of \mathcal{E} as $\alpha \rightarrow 0$. By Lemma 2.5, this problem has a unique solution f^α for all $\alpha > 0$.

The formal limit F of f^α as $\alpha \rightarrow 0$ is the solution of the classical SHE (CSHE) model:

$$N(\varepsilon)\partial_t F - \tilde{\nabla} \cdot (D \tilde{\nabla} F) = 0 \quad (2.11)$$

$$F(0, x, \varepsilon) = F_{in}(x, \varepsilon)$$

$$\tilde{\nabla} = \nabla_x - \nabla_x V \partial_\varepsilon, \quad (2.12)$$

$$D = \mathcal{P}(\mathcal{C}_{el}^{-1}(p) \otimes p) = \frac{|p|^2}{4\pi} \int_{\mathbb{S}^2} \mathcal{C}_{el}^{-1}(\omega) \otimes \omega d\omega.$$

More precisely, the sequence $(f^\alpha)_\alpha$ can be rigorously proved to converge weakly in $L^\infty((0, T), L^2_{x,p})$ to a limit $F \in L^\infty((0, T), \mathcal{E})$ which is a weak solution of (2.11), and $F \geq 0$. Moreover, the following expression

$$H_{CSHE}(F) = \int F \left(\ln \frac{F}{\mathcal{M}} - 1 \right) N(\varepsilon) d\varepsilon dx$$

is a decreasing function of time.

Proof: The proof of the derivation itself can be found in [7, 15] (formal proof) and [14], for a rigorous proof in the case of a null potential V . When the potential

does not vanish, the proof can be adapted from [19] where the diffusion is driven by particle-wall scattering. \square

An interesting case is when the collision kernel is isotropic: $\mathcal{S}(p, p') = \mathcal{S}(|p|, |p'|)$. Then, setting $\mathcal{S}(|p|, |p|)N(|p|^2/2) = \nu$, the collision operator reads:

$$\mathcal{C}_{el}(f) = \nu (\mathcal{P}f - f) \quad (2.13)$$

and the diffusion matrix is a scalar given by

$$D = \frac{4\pi}{3\nu}(2\varepsilon)^{3/2}. \quad (2.14)$$

Remark 2.7 The Classical SHE model given by equation (2.11) is a degenerate parabolic equation.

Remark 2.8 Note that, in the definition of this operator (2.13), the projection term $\mathcal{P}f$ can be obtained as the minimizer of the classical entropy $H_C(g)$ under the constraint $\mathcal{P}(g - f) = 0$. The definition of a quantum analogue of this relaxation operator in section 4.2 is inspired by this remark. \square

3 Classical collision operators and Quasi-Quantum SHE model

As a first attempt to introduce quantum phenomenology in the SHE model, the Wigner equation can be substituted to the left hand side of the Boltzmann equation (2.1). This is our goal in the present section. First, the Wigner-Boltzmann equation (*i.e.* the Wigner equation with a collisional source term) is introduced. Some notations and properties are given and the resolution of the Cauchy problem for this equation is recalled. Note that in this section, we will focus on the influence of

the quantum transport operator. The scattering phenomena are still modeled by a classical collision operator. We emphasize that this approach lacks consistency, as we use a quantum model for transport and still a classical model for collisions. In order to remedy to this inconsistency, we introduce quantum collision operators in section 4.

The so-called Quasi-Quantum SHE (QQSHE) model is rigorously derived from the Wigner-Boltzmann equation in a diffusion asymptotics. As the Wigner equation, the QQSHE model depends on the Planck constant. The expansion of this model with respect to \hbar is investigated and a focus is made on the QQSHE₂ model, that is, the expanded model up to second order terms in \hbar . This model is of interest since it introduces correction terms to the CSHE model and may lead to a cheap yet accurate way to introduce quantum corrections in classical SHE models.

3.1 The Wigner-Boltzmann equation

Let us introduce the Wigner transform and its properties. All the results of this subsection are given without proof (one can refer to [40] for instance). To any complex number z we associate its complex conjugate \bar{z} . We adopt the following conventions for the Fourier transform \mathcal{F} and the inverse Fourier transform \mathcal{F}^{-1} (in dimension 3)

$$\mathcal{F}(f)(\eta) = \int f(p)e^{-ip\cdot\eta/\hbar}dp, \quad \mathcal{F}^{-1}(g)(p) = \int g(\eta)e^{ip\cdot\eta/\hbar}\frac{d\eta}{(2\pi\hbar)^3}$$

where \hbar is the reduced Planck constant. Let ρ denote a trace class nonnegative hermitian operator on $L^2(\mathbb{R}^3)$ and let $\rho(x, y)$ be its integral kernel. Then its Wigner transform is

$$W[\rho](x, p) = \int_{\mathbb{R}^3} \rho\left(x - \frac{\eta}{2}, x + \frac{\eta}{2}\right) e^{i\eta\cdot p/\hbar}d\eta$$

whereas the Weyl quantization of any symbol $a(x, p)$ defines an operator $\text{Op}(a)$:

$$\text{Op}(a)\phi = (2\pi\hbar)^{-3} \int_{\mathbb{R}^6} a\left(\frac{x+y}{2}, p\right) \phi(y) e^{ip \cdot (x-y)/\hbar} dp dy.$$

Then Op and W are formally inverse operations to one another:

$$\text{Op}(W[\rho]) = \rho \quad ; \quad W[\text{Op}(a)] = a.$$

For any trace class operator ρ , we denote by $\text{Tr } \rho$ its trace and by ρ^\dagger its hermitian adjoint. We summarize some classical properties of Op and W in the following lemma. We recall that an operator K is a Hilbert-Schmidt operator if there exists a kernel $k \in L^2_{x,p}$ such that, for any $\phi \in L^2_{x,p}$, $K(\phi)(y) = \int k(x, y)\phi(x)dx$. We note $K \in \text{HS}$.

Lemma 3.1 (Properties of W and Op)

- (i) The Weyl quantization $\text{Op}(a)$ of a symbol a is a Hilbert-Schmidt operator if and only if a is in $L^2_{x,p}$. Moreover, Op is an isometry from $L^2_{x,p}$ onto HS.
- (ii) An operator ρ is hermitian if and only if $W[\rho]$ is real valued. The Wigner transform W , defined from HS onto $L^2_{x,p}$ is the inverse transform to the Weyl quantization.
- (iii) For two Hilbert-Schmidt operators ρ and σ , the following formula is a consequence of Plancherel's identity

$$\text{Tr} \{\rho\sigma^\dagger\} = \frac{1}{(2\pi\hbar)^3} \int W[\rho] \overline{W[\sigma]} dx dp. \quad (3.1)$$

- (iv) Let $\mathcal{H} = -\frac{\hbar^2}{2}\Delta + V$ denote the particle Hamiltonian. Then, for any Hilbert-Schmidt operator ρ , we formally have

$$\frac{i}{\hbar} W[\mathcal{H}, \rho] = (p \cdot \nabla_x - \theta[V]) (W[\rho]), \quad (3.2)$$

where $\theta[V]$ denotes the pseudodifferential operator associated with the potential $V(x)$:

$$\begin{aligned}\theta[V]f &= \mathcal{F}^{-1} \left(i \frac{V(x + \frac{\eta}{2}) - V(x - \frac{\eta}{2})}{\hbar} \mathcal{F}(f) \right) \\ &= \frac{i}{(2\pi)^3} \int_{\mathbb{R}^6} \frac{V(x + \frac{\hbar}{2}\eta) - V(x - \frac{\hbar}{2}\eta)}{\hbar} f(t, x, p') e^{i(p-p')\cdot\eta} d\eta dp',\end{aligned}\tag{3.3}$$

and $[\rho, \sigma] = \rho\sigma - \sigma\rho$ is the commutator of two operators ρ and σ .

(v) $\text{Op}(|p|^2) = -\hbar^2\Delta$ and, for any symbol s depending only on x , $\text{Op}(s)$ is the s -multiplication operator: $\text{Op}(s)\varphi : x \rightarrow s(x)\varphi(x)$.

Now we recall the link between the Wigner and the von Neumann equations. The density matrix ρ satisfies the von Neumann equation

$$i\hbar\partial_t\rho = [\mathcal{H}, \rho]\tag{3.4}$$

if and only if its Wigner transform $f = W[\rho]$ satisfies the Wigner equation

$$\partial_t f + p \cdot \nabla_x f - \theta[V]f = 0\tag{3.5}$$

as can be seen thanks to Eq. (3.2). The function f cannot be easily interpreted as a distribution function (for instance, it is not necessarily positive), but the classical transport equation $\partial_t f + (p \cdot \nabla_x - \nabla_x V \cdot \nabla_p)f = 0$ can be obtained as the semi-classical limit of the Wigner equation as \hbar tends to 0 (see [40]).

Lemma 3.3 gives some information on the operator $\theta[V]$ if we assume:

Assumption 3.2 *The potential V lies in $W^{2,\infty}(\mathbb{R}^3)$.*

Lemma 3.3 *If the potential V satisfies Assumption 3.2, then*

- (i) $\theta[V]$ is a bounded skew-adjoint operator from $L^2_{x,p}$ to $L^2_{x,p}$,
- (ii) for any function $f \in W^{2,2}(\mathbb{R}_x^3; L^2(\mathbb{R}_p^3))$,

$$\theta[V](f) \in W^{2,2}(\mathbb{R}_x^3, L^2(\mathbb{R}_p^3)),$$

and, for $f \in W^{1,2}(\mathbb{R}_x^3; L^2(\mathbb{R}_p^3))$,

$$\nabla_x \theta[V]f = \theta[\nabla_x V](f) + \theta[V](\nabla_x f),$$

where $\theta[\nabla_x V](f)$ and $\theta[V](\nabla_x f)$ denote respectively the two vectors of components $\theta[\partial_{x_i} V](f)$ and $\theta[V](\partial_{x_i} f)$, for $i = 1, 2, 3$,

(iii) for any function $f \in L_{x,p}^2$ such that $pf \in (L_{x,p}^2)^3$, $p\theta[V](f)$ is in $L_{x,p}^2$,

(iv) for any function $F \in \mathcal{E}$, $\theta[V]F$ belongs to \mathcal{E}^\perp .

Eq. (3.5) does not take collision phenomena into account. In the remainder of section 3 it is assumed that the scattering can be modeled through a classical elastic collision operator. Therefore, the collision operator is still \mathcal{C}_{el} , as defined in (2.8). This leads to the following Wigner-Boltzmann equation (after rescaling):

$$\alpha \partial_t f^\alpha + (p \cdot \nabla_x - \theta[V]) f^\alpha = \frac{1}{\alpha} \mathcal{C}_{el}(f^\alpha) \quad (3.6)$$

We denote by Λ the Wigner operator of domain $\mathcal{D}(\Lambda) = \{g \in L_{x,p}^2 : p \cdot \nabla_x g \in L_{x,p}^2\}$ and defined by

$$\begin{aligned} \Lambda : \mathcal{D}(\Lambda) &\rightarrow L_{x,p}^2 \\ g &\rightarrow (p \cdot \nabla_x - \theta[V]) g. \end{aligned}$$

Note that, since $\theta[V]$ is skew-adjoint on $L_{x,p}^2$, so is Λ on $\mathcal{D}(\Lambda)$.

Remark 3.4 The Wigner-Boltzmann equation equipped with the classical relaxation operator \mathcal{C}_{el} does not preserve positivity. In this sense, it is not a consistent quantum model. \square

For the study of the QQSHE model, we introduce the following functional spaces:

$$\mathcal{L}_{N^k}^2 = \left\{ h(x, \varepsilon) - \text{measurable} : \int_{\mathbb{R}_x^3} \int_{\varepsilon > 0} |h(x, \varepsilon)|^2 (N(\varepsilon))^k d\varepsilon dx < \infty \right\}, \quad (3.7)$$

with $N(\varepsilon) = \sqrt{2\varepsilon}$ and $k \in \mathbb{Z}$. So $\mathcal{E} = \mathcal{L}_N^2$.

Now, we give an existence result for the Wigner-Boltzmann equation (3.6).

Lemma 3.5 *Suppose Assumptions 2.4 and 3.2 hold true.*

Then, for any value of the parameter $\alpha > 0$, any initial condition $f_I^\alpha \in \mathcal{D}(\Lambda)$ and any time $T > 0$, there exists a unique solution $f^\alpha \in C^1([0, T]; L^2_{x,p}) \cap C^0([0, T]; \mathcal{D}(\Lambda))$ to the initial value problem (3.6), $f(t = 0, x, p) = f_I^\alpha$.

Proof: This is a straightforward consequence of the classical semigroup theory - see *e.g.* [37] and [51]. Indeed, Λ is a skew-adjoint operator and generates a unitary group by Stone's theorem. Since \mathcal{C}_{el} is a bounded perturbation of Λ , $\mathcal{C}_{el} + \Lambda$ with domain $\mathcal{D}(\Lambda)$ generates a group of operators. \square

3.2 The Quasi-Quantum SHE model (QQSHE)

This section is dedicated to the investigation of the limit $\alpha \rightarrow 0$ in (3.6). The collision phenomena are modeled by the collision operator \mathcal{C}_{el} defined by (2.13). For the sake of simplicity, we assume that the collision frequency ν is constant. The main result of this section is

Theorem 3.6 *Assumptions 2.4 and 3.2 are supposed to hold true.*

Let $f_I^\alpha \in L^2_{x,p}$ be a convergent sequence such that the limit f_I be in \mathcal{E} . We note $F_I(x, |p|^2/2) = f_I(x, p)$. Therefore, F_I is in \mathcal{L}^2_N . We assume that the collision frequency ν is constant.

Let f^α denote the solution of (3.6), with initial condition $f^\alpha(t = 0, x, p) = f_I^\alpha(x, p)$, and with the relaxation operator $\mathcal{C}_{el}(f) = \nu(\mathcal{P}(f) - f)$. Then, as $\alpha \rightarrow 0$, the sequence $(f^\alpha)_{\alpha>0}$ converges (up to the extraction of a subsequence) weakly in $L^2(0, T; L^2_{x,p})$ to a limit $f \in L^2(0, T; \mathcal{E})$. We note $F(t, x, |p|^2/2) = f(t, x, p)$, so that $F \in L^2(0, T; \mathcal{L}^2_N)$. In addition, F is a weak solution of:

$$\partial_t F - \frac{1}{\nu} \mathcal{P}(\Lambda(\Lambda(F))) = 0, \quad (3.8)$$

$$F(t = 0, x, \varepsilon) = F_I(x, \varepsilon). \quad (3.9)$$

Remark 3.7 If the collisions are modeled by the more general collision operator (2.8), then one can prove that the limit equation satisfied by F is

$$\partial_t F - \mathcal{P}(\Lambda(\mathcal{C}_{el}^{-1}(\Lambda(F)))) = 0, \quad (3.10)$$

under the condition that the following set of test functions is dense in $L^\infty(0, T; \mathcal{L}_N^2)$:

$$\mathbb{H} = \{\varphi \in W^{1,\infty}(0, T; C_c^\infty(\mathbb{R}^3 \times \mathbb{R}^+)) : \mathcal{P}(\Lambda(\mathcal{C}_{el}^{-1}(\Lambda\varphi))) \in L^\infty(0, T; \mathcal{L}_N^2)\}.$$

This condition is obviously fulfilled when $\mathcal{C}_{el} = \nu(\mathcal{P}f - f)$.

It is possible to insert the expression of Λ into (3.8) (or (3.10)), in order to get a more explicit form of the equation. However, this expression is quite complicated and not very illuminating. We shall derive an explicit expression after using an expansion of Λ in powers of \hbar at section 3.3 below. \square

Remark 3.8 The quantum (Wigner) transport operator does not preserve the classical entropy. Therefore, there is no (obvious) classical entropy dissipation for the Quasi Quantum SHE model. Also, the classical relaxation operator \mathcal{C}_{el} does not decay the quantum entropy introduced below in section 4. This leaves little hope to find a simple entropic structure for this model, at least in the framework presented in this paper.

We have to mention that, unlike the Classical SHE model, the QQSHE model has not a clear parabolic (or even degenerate parabolic) structure. Indeed, the Wigner transport operator is a pseudo-differential operator, not a true partial differential operator.

Last, but not least, the quantum relevance of this model is weak since there is no indication whether it admits positive solutions (in the sense of operator positivity). \square

Proof: We start from (3.6). We multiply by f^α and integrate with respect to t , x and p . This yields

$$\|f^\alpha(t)\|_{L_{x,p}^2}^2 + \frac{1}{\alpha^2} \int_0^t \|\mathcal{P}^\perp f^\alpha(s)\|_{L_{x,p}^2}^2 ds = \|f_I^\alpha\|_{L_{x,p}^2}^2. \quad (3.11)$$

Therefore, the sequence (f^α) is bounded in $L_{x,p}^2$ since (f_I^α) is bounded. There exists f in $L^\infty(0, T; L_{x,p}^2)$ such that $f^\alpha \rightharpoonup f$ weakly $*$ in $L^\infty(0, T; L_{x,p}^2)$. Moreover, the same estimate (3.11) shows that $\mathcal{P}^\perp f^\alpha$ tends strongly to 0 as $\alpha \rightarrow 0$ in the same space. Consequently, the limit f belongs to \mathcal{E} and we can note $F(t, x, |p|^2/2) = f(t, x, p)$.

The Wigner-Boltzmann equation can be written in a weak form, by introducing the following set of test functions:

$$\mathcal{S} = \{\varphi \in W^{1,\infty}(0, T; L_{x,p}^2) \cap L^\infty(0, T; \mathcal{D}(\Lambda)) : \varphi(T, x, p) = 0\}.$$

The weak solutions of (3.6) satisfy

$$\forall \varphi \in \mathcal{S} \quad \int_{[0,T] \times \mathbb{R}^6} f^\alpha \left(\partial_t \varphi + \frac{1}{\alpha} \Lambda \varphi + \frac{1}{\alpha^2} \mathcal{C}_{el} \varphi \right) dt dx dp = \int_{\mathbb{R}^6} f_I^\alpha \varphi(0, x, p) dx dp. \quad (3.12)$$

In order to prove that F is a weak solution of (3.8), let us introduce a test function $\Phi(t, x, \varepsilon)$ for this equation, in $W^{1,\infty}(0, T; C_c^\infty(\mathbb{R}^3 \times \mathbb{R}^+))$. Obviously the function $\varphi_1(t, x, p)$ defined by $\varphi_1(t, x, p) = \Phi(t, x, |p|^2/2)$ belongs to \mathcal{S} and can be taken as a test function in (3.12). We consider the asymptotic behaviour of each term in (3.12) as $\alpha \rightarrow 0$, in this special case where the test function φ_1 is a function of $(t, x, |p|^2/2)$. The weak convergence of f^α implies

$$\int f^\alpha \partial_t \varphi_1(t, x, p) dt dx dp \rightarrow \int N(\varepsilon) F(t, x, \varepsilon) \partial_t \Phi(t, x, \varepsilon) dt dx d\varepsilon$$

and

$$\int f_I^\alpha \varphi_1(0, x, p) dx dp \rightarrow \int N(\varepsilon) F_I(x, \varepsilon) \Phi(0, x, \varepsilon) dx d\varepsilon.$$

On the other hand, since $\varphi_1(t, \cdot, \cdot) \in \mathcal{E}$, necessarily $\int f^\alpha \mathcal{C}_{el} \varphi_1 dt dx dp = 0$.

Let us decompose f^α as follows:

$$f^\alpha = F^\alpha + \alpha g^\alpha,$$

with $F^\alpha = \mathcal{P}f^\alpha$ and $g^\alpha = \mathcal{P}^\perp f^\alpha / \alpha$. According to Lemma 3.3 (iv), $\Lambda\varphi_1$ lies in \mathcal{E}^\perp .

Therefore, $\int F^\alpha \Lambda\varphi_1 dt dx dp = 0$ since $F^\alpha \in \mathcal{E}$ and

$$\frac{1}{\alpha} \int f^\alpha \Lambda\varphi_1 dt dx dp = \int g^\alpha \Lambda\varphi_1 dt dx dp. \quad (3.13)$$

We are thus led to investigate the behaviour of g^α as $\alpha \rightarrow 0$. According to Eq. (3.11), and using the definition of g^α , we have

$$\int_0^t \|g^\alpha(s)\|_{L_{x,p}^2} ds \leq C.$$

Therefore, there exists g such that $g^\alpha \rightharpoonup g$ weakly $*$ in $L^\infty(0, T; L_{x,p}^2)$ and,

$$\frac{1}{\alpha} \int f^\alpha \Lambda\varphi_1 dt dx dp = \int g^\alpha \Lambda\varphi_1 dt dx dp \rightarrow \int g \Lambda\varphi_1 dt dx dp \quad (3.14)$$

as $\alpha \rightarrow 0$. It remains to relate the last integral in (3.14) to F .

To this aim, we come back to (3.12), that we write with another particular test function φ_2 (specified below). Eq. (3.12) can be written in terms of g^α and F^α . Since the sequences F^α and g^α are bounded, keeping only the leading order terms in this equation leads to

$$\int g^\alpha \mathcal{C}_{el} \varphi_2 dt dx dp = - \int F^\alpha \Lambda\varphi_2 dt dx dp + \mathcal{O}(\alpha),$$

or, letting $\alpha \rightarrow 0$,

$$\int g \mathcal{C}_{el} \varphi_2 dt dx dp = - \int F \Lambda\varphi_2 dt dx dp. \quad (3.15)$$

Now, by choosing

$$\varphi_2 = (\mathcal{C}_{el})^{-1}(\Lambda\varphi_1),$$

we deduce that the last integral in (3.14) can be rewritten

$$\int g \Lambda \varphi_1 dt dx dp = \int g \mathcal{C}_{el} \varphi_2 dt dx dp$$

and straightforward calculations lead to

$$\int g \Lambda \varphi_1 dt dx dp = - \int N F \mathcal{P} (\Lambda ((\mathcal{C}_{el})^{-1}(\Lambda \varphi_1))) dt dx d\varepsilon.$$

Finally, we get

$$\int N F (\partial_t \Phi - \mathcal{P} (\Lambda ((\mathcal{C}_{el})^{-1}(\Lambda \varphi_1)))) dt dx d\varepsilon = \int N F_I \Phi(0, x, \varepsilon) dx d\varepsilon \quad (3.16)$$

which is obviously the weak form of (3.10). It remains to check that this formal identification can be made rigorous. Namely, we have to prove that, if $\Phi \in W^{1,\infty}(0, T; C_c^\infty(\mathbb{R}^3 \times \mathbb{R}^+))$, then $\varphi_2 = (\mathcal{C}_{el})^{-1}(\Lambda \varphi_1)$ is an admissible test function for (3.12). By Lemma 3.3 (under Assumption 3.2), it is an easy task, since we have

$$(\mathcal{C}_{el})^{-1}(\Lambda \varphi_1) = -\frac{1}{\nu} \Lambda \varphi_1.$$

□

3.3 The QQSHE₂ model: quantum corrections to the classical SHE model

The explicit form of the diffusion term $\mathcal{P}(\Lambda(\Lambda F)) N(\varepsilon)/\nu$ in (3.8) is not easy to handle. As in [20] we give the expansion of this model in \hbar , up to second order terms. This leads to the classical SHE model enriched with quantum correction terms.

In the remainder of this paper, when a function F depends on p through the energy $|p|^2/2$ only, we note equally $F(|p|^2/2) = F(p)$ when the context is clear.

The Wigner transport operator Λ depends on the reduced Planck constant. At usual macroscopic scales, this constant is negligible and the transport operator Λ can be expanded in powers of \hbar . Formally, one has

$$\Lambda = L + \hbar^2 L^{(2)} + \mathcal{O}(\hbar^4) \quad (3.17)$$

where $L = p \cdot \nabla_x - \nabla_x V \cdot \nabla_p$ is the classical transport operator and $L^{(2)}$ is a third order differential operator given by

$$L^{(2)} = \frac{1}{24} \nabla_x^{\otimes 3} V \dot{\nabla}_p^{\otimes 3}.$$

Here the third order tensors are defined as $(\nabla_x^{\otimes 3})_{i,j,k} = \partial_{x_i, x_j, x_k}^3$ (and analogously for $\nabla_p^{\otimes 3}$) and $\dot{\nabla}_p^{\otimes 3}$ denotes the third order tensor product. Formula (3.17) gives the leading and second order terms of the so-called Wigner-Moyal expansion (see [46]).

Then the diffusion term becomes

$$N(\varepsilon) \mathcal{P}(\Lambda(\Lambda F)) = N(\varepsilon) \mathcal{P}(L(LF)) + \hbar^2 N(\varepsilon) (\mathcal{P}(L^{(2)}(LF)) + \mathcal{P}(L(L^{(2)}F))) + \mathcal{O}(\hbar^4).$$

Note that $\mathcal{P}(L(LF))$ is the diffusion term that is involved in the CSHE model (2.11), (2.14). Indeed, when F is a function of the position and energy only $LF = p \cdot \tilde{\nabla} F$, where $\tilde{\nabla}$ is the “twisted” gradient operator defined at (2.12). Therefore, $L(LF) = p^{\otimes 2} : \tilde{\nabla}^{\otimes 2} F - \nabla_x V \cdot \tilde{\nabla} F$. Applying projector \mathcal{P} yields

$$N(\varepsilon) \mathcal{P}(L(LF)) = 4\pi \frac{(2\varepsilon)^{3/2}}{3} \tilde{\nabla} \cdot \tilde{\nabla} F - 4\pi (2\varepsilon)^{1/2} \nabla_x V \cdot \tilde{\nabla} F$$

and one can check that the right hand side of this equation can be written

$$4\pi \tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{3/2}}{3} \tilde{\nabla} F \right)$$

which is the diffusion term in the classical SHE model.

For the computation of the other terms, we refer the reader to Appendix A. They are summarized in the following formal Lemma:

Lemma 3.9 *We assume that the collision operator is given by (2.13). Up to second order terms in \hbar , the QQSHE model can be formally approached by the following QQSHE₂ model (in the case where ν is a constant independent of ε):*

$$N(\varepsilon)\partial_t F - \frac{4\pi\tilde{\nabla}}{\nu} \cdot \left(\frac{(2\varepsilon)^{3/2}}{3} \tilde{\nabla} F \right) - \frac{4\pi\hbar^2}{24\nu} \left\{ \frac{\partial^2}{\partial\varepsilon^2} \left(\frac{(2\varepsilon)^{5/2}}{5} \nabla_x(\Delta V) \cdot \partial_\varepsilon \tilde{\nabla} F \right) + \frac{\partial}{\partial\varepsilon} \tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{5/2}}{5} \nabla_x(\Delta V) \partial_\varepsilon^2 F \right) \right\} = 0. \quad (3.18)$$

Remark 3.10 Compared with the CSHE model (2.11), additional terms involving fourth order derivatives appear. They are multiplied by factors involving third order derivatives of the potential, which is natural since these factors appear in the first correction to the classical limit in the Wigner-Moyal expansion [46]. Also, these fourth order derivatives of F involve cross-diffusion terms mixing space and energy derivatives. This is to be related with the cross-diffusion terms that appear in the Fokker-Planck equation used in [4]. \square

Remark 3.11 Given that the coefficients of the fourth order derivatives have no fixed sign, one can wonder about the stability and well-posedness of this model. As for the QQSHE model, there is no clear entropic structure for the QQSHE₂ model. Therefore, no clear indication is given why this model should be well-posed. A linearized stability analysis of this model is in progress to try to answer this question. If the model is found linearly stable, there is good hope that it can be used to efficiently simulate quantum semiconductor devices numerically. \square

4 Quantum collision operators

All the results given in the following section are formal. In Section 3, the SHE models are of a hybrid type since they are derived from a microscopic equation

with a quantum transport term and a classical collision operator. To remedy to this inconsistency, we need to develop a notion of quantum collision operator which allows us to perform the program leading to SHE-type models.

An important property of the collision operators used in classical kinetic theory is the entropy dissipation. Therefore, a natural requirement of a quantum collision operator \mathcal{Q} is that it dissipates quantum entropy and that a quantum kinetic equation such as the Wigner-Boltzmann equation

$$\partial_t f + p \cdot \nabla_x f - \theta[V]f = \mathcal{Q}(f) \quad (4.1)$$

satisfies a quantum analogue to Lemma 2.1.

The collision operator \mathcal{Q} will be derived as a quantum counterpart of the classical electron-phonon collision operator (or its elastic approximation). Therefore, the equilibrium states of this quantum operator will be “quantum” Maxwellian, as the classical operator had (“classical”) Maxwellian equilibria. Consequently, the quantum relative entropy associated with the Von Neumann equation (3.4) is defined by $H_Q(\rho) = \text{Tr} \{ \rho(\ln \rho - 1 + \mathcal{H}) \}$ where $\mathcal{H} = -(\hbar^2/2)\Delta + V$ is the particle Hamiltonian. Lemma (3.1) allows to deduce the expression of quantum entropy in the Wigner framework by

$$H_Q(f) = \frac{1}{(2\pi\hbar)^3} \int f \left(\mathcal{L}n(f) + \frac{|p|^2}{2} + V - 1 \right) dpdx, \quad (4.2)$$

where the “quantum logarithm” $\mathcal{L}n$ is defined by

$$\mathcal{L}n(f) = W [\ln (\text{Op}(f))],$$

assuming that $\text{Op}(f) > 0$. Analogously, we define the “quantum exponential” and the quantum Maxwellian \mathcal{M}_{ax} respectively by

$$\mathcal{E}xp(f) = W [\exp (\text{Op}(f))],$$

$$\mathcal{M}_{\max}(x, p) = W \left[\exp \left(\text{Op} \left(-\frac{|p|^2}{2} - V(x) \right) \right) \right] = \mathcal{E}_{\text{xp}}(-|p|^2/2 - V).$$

Note that \mathcal{L}_{n} and \mathcal{E}_{xp} are formal inverses and that $-|p|^2/2 - V = \mathcal{L}_{\text{n}}(\mathcal{M}_{\max}(x, p))$.

Then (4.2) is equivalently written (up to a constant multiplier $(2\pi\hbar)^2$)

$$H_Q(f) = \int f (\mathcal{L}_{\text{n}}(f) - \mathcal{L}_{\text{n}}(\mathcal{M}_{\max}) - 1) dpdx$$

and appears as the quantum relative entropy with respect to quantum Maxwellian steady states. The following Lemma gives a criterion on \mathcal{Q} for Eq. (4.1) to be consistent with the quantum entropy H_Q .

Lemma 4.1 *Let \mathcal{Q} in (4.1) be such that, for any function g , we have:*

$$- \int \mathcal{Q}(g) (\mathcal{L}_{\text{n}}(g) - \mathcal{L}_{\text{n}}(\mathcal{M}_{\max})) dx dp \geq 0 \quad (4.3)$$

Then, if f is a solution of Eq. (4.1), the associated quantum entropy satisfies:

$$\frac{dH_Q(f)}{dt} \leq 0. \quad (4.4)$$

Proof: To begin with, we recall that H_Q is Gâteaux differentiable and its Gâteaux derivative at f in the direction δf is (see [22]):

$$H'_Q(f)\delta f = (2\pi\hbar)^3 \text{Tr} \{ (\ln \text{Op}(f) + \mathcal{H}) \text{Op}(\delta f) \}$$

or,

$$H'_Q(f)\delta f = \int \left(\mathcal{L}_{\text{n}}f + \frac{|p|^2}{2} + V \right) \delta f dpdx.$$

Therefore, if f is a solution of (4.1),

$$\begin{aligned} \frac{dH_Q(f)}{dt} &= \int \left(\mathcal{L}_{\text{n}}f + \frac{|p|^2}{2} + V \right) \partial_t f dpdx \\ &= - \int \left(\mathcal{L}_{\text{n}}f + \frac{|p|^2}{2} + V \right) \Lambda f dpdx - \int \left(\mathcal{L}_{\text{n}}f + \frac{|p|^2}{2} + V \right) \mathcal{Q}(f) dpdx \\ &= - \int \left((W[\ln(\text{Op}(f))] + W[\mathcal{H}]) \frac{i}{\hbar} W[\mathcal{H}\text{Op}(f) - \text{Op}(f)\mathcal{H}] \right) dpdx \\ &\quad - \int (\mathcal{L}_{\text{n}}(f) - \mathcal{L}_{\text{n}}(\mathcal{M}_{\max})) \mathcal{Q}(f) dpdx \end{aligned} \quad (4.5)$$

thanks to Lemma (3.1) (iv). Now, using (3.1) (iii), the first integral on the right hand side can be written

$$(2\pi)^3 i\hbar^2 \text{Tr} \{(\ln(\text{Op}(f)) + \mathcal{H}) [\mathcal{H}, \text{Op}(f)]\}$$

or, using the cyclicity of the trace,

$$(2\pi)^3 i\hbar^2 \text{Tr} \{[\text{Op}(f), \ln(\text{Op}(f))] \mathcal{H} + [\mathcal{H}, \mathcal{H}] \text{Op}(f)\}$$

and this trace is obviously null. Finally, the second integral on the right-hand side of (4.5) is nonnegative according to (4.3), which completes the proof. \square

Consequently, after [23], what is meant in this paper by quantum collision operators is a class of collision operators \mathcal{Q} that satisfy the following formal properties: for any function $f(x, p)$,

$$\textit{Mass conservation: } \int \mathcal{Q}(f)(p) dx dp = 0,$$

$$\textit{Entropy dissipation: } - \int \mathcal{Q}(f) (\mathcal{L}n(f) - \mathcal{L}n(\mathcal{M}_{\text{ax}})) dx dp \geq 0.$$

4.1 The Quantum electron-phonon collision operator

In this section, quantum counterparts of the classical collision operator $\mathcal{C}_{e\varphi}$ and of its elastic approximation \mathcal{C}_{el} are introduced. They may lead to possibly interesting quantum models for electron-phonon scattering. Moreover, the derivation of a Quantum SHE model in section 5 is performed from a quantum kinetic equation with a relaxation collision operator which can be understood as a relaxation approximation of the operators studied in this section.

Keeping Lemma 4.1 in mind, we introduce the following quantum version of the electron-phonon collision operator $\mathcal{C}_{e\varphi}$ described in Section 2.2 (we recall that β is the phonon energy in scaled variables):

$$\mathcal{Q}_{e\varphi}(f) = \int \mathcal{S}(p, p') [\delta(\varepsilon' - \varepsilon - \beta) + \delta(\varepsilon' - \varepsilon + \beta)] \left(\frac{\mathcal{A}(f)'}{M'} - \frac{\mathcal{A}(f)}{M} \right) dp' \quad (4.6)$$

where

$$\mathcal{A}(f) = \exp W[\ln \text{Op}(f)] = \exp \mathcal{L}n f, \quad (4.7)$$

namely $\mathcal{L}n f = \ln \mathcal{A}(f)$ where \ln is the ordinary logarithm. Note that it is not clear what conditions f should satisfy for $\mathcal{A}(f)$ to be a well defined function. Therefore, the definition of $\mathcal{Q}_{e\varphi}$ is purely formal at this point and all the results stated in this Section are formal.

However, we claim that this operator is a natural extension of the classical phonon operator to quantum systems, and that it is consistent with quantum entropy relaxation. Indeed, we have:

Proposition 4.2 *The collision operator $\mathcal{Q}_{e\varphi}$ defined by (4.6) satisfies the following properties:*

- (i) *Mass conservation: $\int \mathcal{Q}_{e\varphi}(f) dp = 0$ for any measurable function f .*
- (ii) *Equilibrium states: for any measurable function $f(x, p)$, we have $\mathcal{Q}_{e\varphi}(f) = 0$ if and only if*

$$f(x, p) = \mathcal{E}xp \left(\frac{|\cdot|^2}{2} + \ln F \left(\frac{|\cdot|^2}{2} \right) \right) (x, p) = W \left[\exp \left(-\frac{\hbar^2}{2} \Delta + \text{Op}(\ln F) \right) \right] (x, p)$$

where $F = F(\varepsilon)$ is such that $F(\varepsilon + \beta) = F(\varepsilon)$.

- (iii) *Entropy dissipation: $-\int \mathcal{Q}_{e\varphi}(f) (\mathcal{L}n(f) - \mathcal{L}n(\mathcal{M}_{\text{ax}})) dp \geq 0$ for any function f .*

Proof: The mass conservation follows from the symmetry of $\mathcal{S}(p, p')$. The equilibria of operator $\mathcal{Q}_{e\varphi}$ can be easily deduced from those of operator $\mathcal{C}_{e\varphi}$ by remarking that $\mathcal{Q}_{e\varphi}(f) = \mathcal{C}_{e\varphi}(\mathcal{A}(f))$. On the other hand, it follows from the symmetry of \mathcal{S} that

$$\begin{aligned} & - \int \mathcal{Q}_{e\varphi}(f) (\mathcal{L}n(f) - \mathcal{L}n(\mathcal{M}_{\text{ax}})) dp = \\ & \frac{1}{2} \int \mathcal{S}(p, p') (\delta_+ + \delta_-) \left(\frac{\mathcal{A}(f)'}{M'} - \frac{\mathcal{A}(f)}{M} \right) \left(\ln \frac{\mathcal{A}(f)'}{M'} - \ln \frac{\mathcal{A}(f)}{M} \right) dp dp' dx \end{aligned}$$

which is nonnegative since \ln is an increasing function. \square

Like in the case of the classical electron-phonon scattering, we are interested in the elastic limit $\beta \rightarrow 0$ of the operator $\mathcal{Q}_{e\varphi}$. More precisely, we let ω_0 tend to zero and get:

$$\mathcal{Q}_{el}(f)(p) = N(|p|^2/2) \left\{ \mathcal{P} \left(\tilde{\mathcal{S}}(p, \cdot) \mathcal{A}(f)(\cdot) \right) - \mathcal{P} \left(\tilde{\mathcal{S}}(p, \cdot) \right) \mathcal{A}(f)(p) \right\}, \quad (4.8)$$

where $\tilde{\mathcal{S}}$ is defined as in section 2.2 by formula (2.9). We drop the tildas in the remainder of the paper. This operator has the properties of a quantum collision operator:

Proposition 4.3 *The collision operator \mathcal{Q}_{el} defined by (4.8) satisfies the following properties:*

- (i) *Mass conservation:* $\int \mathcal{Q}_{el}(f) dp = 0$ for any measurable function f .
- (ii) *Equilibrium states:* for any measurable function $f(x, p)$, we have $\mathcal{Q}_{el}(f) = 0$ if and only if there exists a function $\lambda(x, \varepsilon)$ of position and energy only such that

$$f(x, p) = \mathcal{E}xp \left(\tilde{\lambda} \right) (x, p),$$

where $\tilde{\lambda}(x, p) = \lambda(x, |p|^2/2)$.

- (iii) *Entropy dissipation:* $-\int \mathcal{Q}_{el}(f) (\mathcal{L}n(f) - \mathcal{L}n(\mathcal{M}_{ax})) dp \geq 0$ for any function f .

Remark 4.4 Note that f , unlike λ , is *not* a function of the energy only in general. Indeed, it is not clear that the quantum exponential of a function of position and energy $(x, \varepsilon(p))$ remains a function of $(x, \varepsilon(p))$ (with $\varepsilon(p) = |p|^2/2$). \square

Proof: Mass conservation and entropy dissipation can be proven in the same way as for $\mathcal{Q}_{e\varphi}$. For (ii), we consider

$$\begin{aligned} -\int \mathcal{Q}_{el}(f)(p) \mathcal{A}(f)(p) dp &= \frac{1}{2} \int \delta \left(\frac{|p'|^2}{2} - \frac{|p|^2}{2} \right) \mathcal{S}(p, p') (\mathcal{A}(f)(p') - \mathcal{A}(f)(p))^2 dp' dp \\ &\geq 0, \end{aligned}$$

where \mathcal{A} is defined by (4.7).

Obviously, if $Q_{el}(f) = 0$, then one necessarily has $\mathcal{A}(f)(x, p) = \mathcal{A}(f)(x, p')$ whenever $|p| = |p'|$. Therefore, $\mathcal{A}(f)$ is a function of x and $|p|^2/2$ only. Consequently, $\ln \mathcal{A}(f)$ depends only on $|p|^2/2$ too and, finally, one can set $\lambda(\varepsilon) = \ln \mathcal{A}(f) = \mathcal{L}nf$, or $f = \mathcal{E}xp\lambda$. \square

4.2 The quantum relaxation operator

In classical kinetic theory, an important class of collision operators is constituted by the relaxation operators. The mathematical study of these operators is simpler than for Boltzmann-like collision operators although they share many important properties with them, such as entropy dissipation, mass conservation and the expression of their equilibrium states.

The task in this section is to introduce a consistent notion of quantum relaxation operator that satisfies properties (i), (ii) and (iii) of Proposition 4.3. To this aim, we introduce the following minimization problem:

Given f , find \mathcal{E}_f such that:

$$H_Q(\mathcal{E}_f) = \text{Min} \{H_Q(g) / \mathcal{P}(f - g) = 0\}. \quad (4.9)$$

Assuming that, for f in a suitable space, a solution \mathcal{E}_f to this problem exists, we set:

$$\mathcal{Q}_{\text{rel}}(f) = \nu(\mathcal{E}_f - f), \quad (4.10)$$

where ν is assumed to be constant in the sequel.

It remains to prove that such an operator has the required properties. We have:

Proposition 4.5 *The collision operator \mathcal{Q}_{rel} defined by (4.10) satisfies the following properties:*

(i) *Mass conservation:* $\int \mathcal{Q}_{\text{rel}}(f) dp = 0$ for any measurable function f .

(ii) *Equilibrium states:* for any measurable function $f(x, p)$, we have $\mathcal{Q}_{\text{rel}}(f) = 0$ if and only if there exists a function $\lambda(x, \varepsilon)$ of x and the energy only such that

$$f(x, p) = \mathcal{E}xp(\tilde{\lambda})(x, p),$$

where $\tilde{\lambda}(x, p) = \lambda(x, |p|^2/2)$.

(iii) *Entropy dissipation:* $-\int \mathcal{Q}_{\text{rel}}(f) (\mathcal{L}n(f) - \mathcal{L}n(\mathcal{M}_{\text{ax}})) dp \geq 0$ for any function f .

Before proving Proposition 4.5, we state an important property of the solutions of the minimization problem (4.9).

Lemma 4.6 *Let f be a function such that a solution of the minimization problem (4.9) exists. We denote such a solution by \mathcal{E}_f . Then, there exists a function $\lambda(x, \varepsilon)$ such that*

$$\mathcal{E}_f(x, p) = \mathcal{E}xp(\lambda)(x, p).$$

Proof: Since \mathcal{E}_f is the minimizer of $H_Q(g)$ under the constraint $\mathcal{P}(f - g) = 0$, there exists a Lagrange multiplier $\mu(x, \varepsilon)$ such that $H'_Q(f)g + \mu\mathcal{P}(g) = 0$ for all g . This means that, for all g ,

$$\int \left(\mathcal{L}n(f) + \frac{|p|^2}{2} + V - \mu(x, |p|^2/2) \right) g(x, p) dp dx = 0,$$

that is: $f = \mathcal{E}xp(\lambda(x, \varepsilon))$ with $\lambda(x, \varepsilon) = \mu(x, \varepsilon) - \varepsilon - V(x)$. □

Proof of Proposition 4.5: Point (i) is obvious since the definition of \mathcal{E}_f implies that $\mathcal{P}(f - \mathcal{E}_f) = 0$. Point (ii) is a straightforward consequence of Lemma 4.6. The proof of point (iii) is inspired from [20]. We introduce

$$\Gamma : \gamma \in [0, 1] \rightarrow \int_{\mathbb{R}^6} \nu(x, \varepsilon) h((1 - \gamma)\mathcal{E}_f + \gamma f) dx dp$$

with $h : f \rightarrow f(\mathcal{L}n f - 1 + |p|^2/2 + V)$. Deriving Γ by a chain rule yields

$$\frac{d\Gamma}{d\gamma}(\gamma) = \int_{\mathbb{R}^6} \nu(x, \varepsilon_p) (f - \mathcal{E}_f) (\mathcal{L}n((1 - \gamma)\mathcal{E}_f + \gamma f) + |p|^2/2 + V) dx dp.$$

The convexity of h implies that Γ is also convex so that $(d\Gamma/d\gamma)(1) \geq \Gamma(1) - \Gamma(0)$, which in turn gives

$$- \int \mathcal{Q}_{\text{rel}}(f) (\mathcal{L}n(f) + |p|^2/2 + V) dx dp \geq \nu (H_Q(f) - H_Q(\mathcal{E}_f)) \geq 0$$

since \mathcal{E}_f is a minimizer of H_Q and ν is a constant. \square

Before turning to the derivation of a fully quantum SHE type model, it is important to underline that the collisional Wigner equation equipped with relaxation type operator \mathcal{Q}_{rel} is a consistent quantum model in the sense that it (formally) preserves positivity. Precisely, the following proposition holds true.

Proposition 4.7 *Let the initial datum f_I be positive (in the sense of operators, i.e. $\rho_I = \text{Op}(f_I)$ is a positive operator). If the following initial value problem*

$$\partial_t f + \Lambda f = \mathcal{Q}_{\text{rel}} f, \quad f(t = 0, x, p) = f_I(x, p)$$

has a solution $f(t, x, p)$, then this solution is positive (i.e. $\rho(t) = \text{Op}(f)(t)$ is a positive operator) for all time.

Proof: The proof is very close to the proof of Lemma 2.1 in [20]. We just emphasize on the positivity of operator $\text{Op}(\mathcal{E}_f)$. Indeed, according to Lemma 4.6, to any given function f there can be associated an energy dependent function λ_f such that

$$\mathcal{E}_f = \mathcal{E} \exp(\lambda_f).$$

Consequently, $\text{Op}(\mathcal{E}_f) = \text{Op}(W(\exp \text{Op}(\lambda_f))) = \exp \text{Op}(\lambda_f)$ which obviously is a positive operator. \square

This quantum relaxation collision operator will be used for the derivation of the full quantum SHE model. Note that at this point, the existence of a minimizer for (4.9) is an open problem.

5 The full Quantum SHE model (QSHE)

In this section, we formally investigate the limit $\alpha \rightarrow 0$ in the following rescaled Wigner-Quantum relaxation equation

$$\alpha \partial_t f^\alpha + \Lambda f^\alpha = \frac{1}{\alpha} \mathcal{Q}_{\text{rel}}(f^\alpha), \quad (5.1)$$

where we recall that $\Lambda = p \cdot \nabla_x - \theta[V]$ is the Wigner operator. In the sequel, we assume that

Assumption 5.1 *For any given function f , there exists a solution \mathcal{E}_f to the minimization problem (4.9), and this solution is unique.*

The following formal result holds:

Theorem 5.2 *If (5.1) admits a solution f^α for all α , and if the so-obtained sequence f^α admits a convergent subsequence, then the limit is denoted by \mathcal{F} and there exists a function λ such that $\tilde{\lambda} : (t, x, p) \rightarrow \lambda(t, x, |p|^2/2)$ satisfies*

$$\begin{aligned} \mathcal{F}(t, x, p) &= \mathcal{E}xp(\tilde{\lambda})(t, x, p) \\ N(\varepsilon) \partial_t \mathcal{P}(\mathcal{E}xp(\tilde{\lambda})) - N(\varepsilon) \mathcal{P}(\Lambda(\frac{1}{\nu} \Lambda(\mathcal{E}xp(\tilde{\lambda})))) &= 0 \end{aligned} \quad (5.2)$$

Furthermore, the quantum entropy decreases with time:

$$\frac{d}{dt} H_{QSHE}(\mathcal{F}) \leq 0, \quad H_{QSHE}(\mathcal{F}) = \int \mathcal{P}(\mathcal{F}) (\lambda + \varepsilon + V - 1) N(\varepsilon) d\varepsilon dx \quad (5.3)$$

Remark 5.3 The main difference between the QQSHE and QSHE models is that the unknown F in the QQSHE model (which is a function of position and energy) is replaced by $\mathcal{E}xp\tilde{\lambda}$ in the QSHE model, where λ is a function of position and energy. This is a true difference since $\mathcal{F} = \mathcal{E}xp\tilde{\lambda}$ is in general *not* a function of position and energy only. This difference makes the QSHE model consistent with *quantum* entropy decay (5.3) rather than classical entropy decay. Again, we do not make this equation more explicit. Indeed, here, it is not possible to make the relation between $\mathcal{E}xp\tilde{\lambda}$ and λ explicit because $\mathcal{E}xp$ is a nonlinear non-local operator. \square

Remark 5.4 Equation (5.2) is closed provided the minimization problem (4.9) is uniquely solvable. Indeed, in this case, there is a one to one correspondence between the intensive quantity λ and the extensive quantity $\mathcal{P}(\mathcal{E}xp\lambda)$. \square

Proof: First, letting $\alpha \rightarrow 0$ in equation (5.1) leads to $\mathcal{Q}_{\text{rel}}(\mathcal{F}) = 0$ so that, according to Proposition 4.5, there exists $\lambda(x, \varepsilon)$ such that $\mathcal{F} = \mathcal{E}xp\tilde{\lambda}$. Now, the Chapman-Enskog expansion of f^α is written

$$f^\alpha = \mathcal{E}_{f^\alpha} + \alpha g^\alpha$$

since f^α is close to the equilibrium when α is small. We assume that \mathcal{E}_{f^α} and g^α are bounded with respect to α in a suitable topology. Then, introducing this expansion in equation (5.1) yields, at first order in α :

$$\mathcal{P}(\partial_t \mathcal{E}_{f^\alpha} + \Lambda g^\alpha) = \mathcal{O}(\alpha) \tag{5.4}$$

and, at zeroth order in α :

$$\Lambda \mathcal{E}_{f^\alpha} = -\nu g^\alpha + \mathcal{O}(\alpha) \tag{5.5}$$

since $\mathcal{Q}_{\text{rel}}(f^\alpha) = \nu(\mathcal{E}_{f^\alpha} - (\mathcal{E}_{f^\alpha} + \alpha g^\alpha)) = -\alpha \nu g^\alpha$. According to (5.5), Eq. (5.4) becomes

$$\mathcal{P}\left(\partial_t \mathcal{E}_{f^\alpha} - \Lambda\left(\frac{1}{\nu}\Lambda \mathcal{E}_{f^\alpha}\right)\right) = \mathcal{O}(\alpha). \tag{5.6}$$

We recall that $\mathcal{E}_{f^\alpha} \rightarrow \mathcal{E} \exp \tilde{\lambda}$ as $\alpha \rightarrow 0$. Letting $\alpha \rightarrow 0$ in (5.6) leads to (5.2). The entropy decay is obtained by taking the limit $\alpha \rightarrow 0$ in (4.4). \square

From now on, we drop the tildas and identify λ to $\tilde{\lambda}$. As in the case of the Quasi-Quantum SHE model, it is interesting to expand the Quantum SHE model in powers of \hbar up to second order terms. We recall that $\Lambda = L + \hbar^2 L^{(2)} + \mathcal{O}(\hbar^4)$ where $L = p \cdot \nabla_x - \nabla_x V \cdot \nabla_p$ is the classical transport operator and $L^{(2)} = (1/24) \nabla_x^{\otimes 3} V : \nabla_p^{\otimes 3}$. However, unlike in the case of the Quasi-Quantum SHE model, here not only does Λ depend on \hbar , but also $\mathcal{E} \exp \lambda$. After [20], the quantum exponential of any function $f(x, p)$ can be written

$$\mathcal{E} \exp f = \exp f [1 + \hbar^2 \mathcal{T} f + \mathcal{O}(\hbar^4)] \quad (5.7)$$

$$\begin{aligned} \mathcal{T} f = & \frac{1}{8} (\nabla_x^{\otimes 2} f : \nabla_p^{\otimes 2} f - \nabla_x \nabla_p f : \nabla_p \nabla_x f + \frac{1}{3} (\nabla_x^{\otimes 2} f : \nabla_p f \nabla_p f \\ & - 2 \nabla_x \nabla_p f : \nabla_p f \nabla_x f + \nabla_p^{\otimes 2} f : \nabla_x f \nabla_x f)). \end{aligned} \quad (5.8)$$

Therefore, the QSHE model is formally approached, up to second order terms, by

$$\begin{aligned} N(\varepsilon) \partial_t F - N(\varepsilon) \mathcal{P} \left(L \left(\frac{1}{\nu} L(F) \right) \right) + \hbar^2 N(\varepsilon) \partial_t [\mathcal{P} (F \mathcal{T}(\ln F))] \\ - \hbar^2 N(\varepsilon) \mathcal{P} \left[\left(L \left(\frac{1}{\nu} L^{(2)} \right) + L^{(2)} \left(\frac{1}{\nu} L \right) \right) (F) - L \left(\frac{1}{\nu} L (F \mathcal{T}(\ln F)) \right) \right] = 0 \end{aligned} \quad (5.9)$$

where we have set $F = \exp \lambda$.

We recall that ν is a constant coefficient. Using the computations already performed to prove Lemma 3.9, we obtain

$$\begin{aligned} N(\varepsilon) \partial_t F - \frac{4\pi}{\nu} \tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{3/2}}{3} \tilde{\nabla} F \right) \\ - \frac{4\pi \hbar^2}{24\nu} \left\{ \frac{\partial^2}{\partial \varepsilon^2} \left(\frac{(2\varepsilon)^{5/2}}{5} \nabla_x(\Delta V) \cdot \partial_\varepsilon \tilde{\nabla} F \right) + \frac{\partial}{\partial \varepsilon} \tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{5/2}}{5} \nabla_x(\Delta V) \partial_\varepsilon^2 F \right) \right\} \\ + \hbar^2 N(\varepsilon) \partial_t [\mathcal{P} (F \mathcal{T}(\ln F))] + \frac{\hbar^2 N(\varepsilon)}{\nu} \mathcal{P} [L (L (F \mathcal{T}(\ln F)))] = 0. \end{aligned}$$

Note that, in this equation, the two first lines correspond to the left hand side of the QQSHE₂ equation (3.18). Other second order terms appear due to the expansion of the quantum exponential $\mathcal{E}x$ into powers of \hbar . Since λ is a function of the position and the energy only, after (5.8) $\mathcal{T}\lambda$ can be written as

$$\begin{aligned} \mathcal{T}\lambda &= \frac{1}{8} \left\{ \Delta\lambda \partial_\varepsilon \lambda + p^{\otimes 2} : (\nabla_x^{\otimes 2} \lambda \partial_\varepsilon^2 \lambda - \nabla_x (\partial_\varepsilon \lambda) \nabla_x (\partial_\varepsilon \lambda)) \right. \\ &\left. + \frac{1}{3} [p^{\otimes 2} : (\nabla_x^{\otimes 2} \lambda (\partial_\varepsilon \lambda)^2 - \partial_\varepsilon (\nabla_x \lambda \nabla_x \lambda) \partial_\varepsilon \lambda + \nabla_x \lambda \nabla_x \lambda \partial_\varepsilon^2 \lambda) + |\nabla_x \lambda|^2 \partial_\varepsilon \lambda] \right\}. \end{aligned} \quad (5.10)$$

According to (5.10), $\mathcal{T}\lambda$ takes the following form

$$\frac{1}{8} (\mathcal{I}_{[\lambda]} + p^{\otimes 2} : \mathcal{J}_{[\lambda]}) \quad (5.11)$$

where

$$\mathcal{I}_{[\lambda]} = \Delta\lambda \partial_\varepsilon \lambda + \frac{1}{3} |\nabla_x \lambda|^2 \partial_\varepsilon \lambda \quad (5.12)$$

$$\begin{aligned} \mathcal{J}_{[\lambda]} &= \nabla_x^{\otimes 2} \lambda \partial_\varepsilon^2 \lambda - \nabla_x (\partial_\varepsilon \lambda) \nabla_x (\partial_\varepsilon \lambda) \\ &+ \frac{1}{3} [\nabla_x^{\otimes 2} \lambda (\partial_\varepsilon \lambda)^2 - \partial_\varepsilon (\nabla_x \lambda \nabla_x \lambda) \partial_\varepsilon \lambda + \nabla_x \lambda \nabla_x \lambda \partial_\varepsilon^2 \lambda]. \end{aligned} \quad (5.13)$$

Therefore, the second order terms in the formal expansion of the QSHE model can be expressed in terms of \mathcal{I} and \mathcal{J} .

Lemma 5.5 *We assume that the collision operator is given by (4.10). Up to second order terms in \hbar , the QSHE model can be formally approached by the following QQSHE₂ model (in the case where ν is a constant):*

$$\begin{aligned} &N(\varepsilon) \partial_t F - \frac{4\pi}{\nu} \tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{3/2}}{3} \tilde{\nabla} F \right) \\ &- \frac{4\pi \hbar^2}{24\nu} \left\{ \frac{\partial^2}{\partial \varepsilon^2} \left(\frac{(2\varepsilon)^{5/2}}{5} \nabla_x (\Delta V) \cdot \partial_\varepsilon \tilde{\nabla} F \right) + \frac{\partial}{\partial \varepsilon} \tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{5/2}}{5} \nabla_x (\Delta V) \partial_\varepsilon^2 F \right) \right\} \\ &+ \frac{4\pi \hbar^2}{8} \left\{ \partial_t \left[F \left(\sqrt{2\varepsilon} \mathcal{I}_{[\ln F]} + \frac{(2\varepsilon)^{2/3}}{3} \text{Trace } \mathcal{J}_{[\ln F]} \right) \right] \right. \\ &\left. + \frac{1}{\nu} \left[\tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{3/2}}{3} \tilde{\nabla} (F \mathcal{I}_{[\ln F]}) \right) + 2 \tilde{\nabla}^{\otimes 2} : \frac{(2\varepsilon)^{5/2}}{15} (F \mathcal{J}_{[\ln F]}) \right] \right\} \end{aligned}$$

$$\tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{5/2}}{3} \tilde{\nabla} (F \text{Trace } \mathcal{J}_{[\ln F]}) \right) \Big] \Big\} = 0,$$

where \mathcal{I} and \mathcal{J} are given by (5.12) and (5.13) respectively, and $\text{Trace } \mathcal{J}$ denotes the trace of the second order tensor \mathcal{J} , namely

$$\text{Trace } \mathcal{J} = \Delta \lambda \partial_\varepsilon^2 \lambda - |\nabla_x (\partial_\varepsilon \lambda)|^2 + \frac{1}{3} (\Delta \lambda (\partial_\varepsilon \lambda)^2 - \partial_\varepsilon (|\nabla_x \lambda|^2) \partial_\varepsilon \lambda + |\nabla_x \lambda|^2 \partial_\varepsilon^2 \lambda). \quad (5.14)$$

Remark 5.6 In this equation, we first find the terms involved in the QQSHE₂ model (3.18) (the first two lines). Then, additional terms arise due to the nonlinear relation between F and $\mathcal{E} \text{xp} \tilde{\lambda}$. They still are fourth order terms, but now they are nonlinear. They still involve crossed derivatives. The same stability questions as for the QQSHE₂ model can be posed for this model, completed by the fact that it is now a nonlinear model. The answer to the stability question is therefore even more complex. That this model can be effective for practical computations is not clear. Probably, a direct numerical resolution of the full QSHE model will be more efficient, as it is the case for Drift Diffusion models (see *e.g.* [29], [30] and [17]). \square

6 Conclusion

In this paper, we have investigated possible quantum extensions of classical SHE (or Fokker-Planck) models. After a review of the derivation of classical SHE models, two possible extensions have been given: one by using a classical operator at the right hand side of a quantum Wigner equation, a second one, by using a quantum version of a relaxation operator. The first approach obviously lacks consistency but gives rise to a seemingly tractable equation. The second approach, although more consistent, gives rise to a rather complex model, the practical effectiveness of which

is not clear. More work is required to settle the question of stability of these models and to try to find more tractable expressions of them.

Appendix

A The QQSHE₂ model

In the sequel, the following identities are needed (a denotes a fourth order tensor and Einstein's convention is used):

$$\mathcal{P}(1) = 1, \quad \mathcal{P}(p) = 0, \quad \mathcal{P}(p^{\otimes 2})(\varepsilon) = \frac{2\varepsilon}{3}\delta, \quad (\text{A.1})$$

$$(\mathcal{P}(p^{\otimes 4}) :: a)(\varepsilon) = \frac{(2\varepsilon)^2}{15} (a_{i,i,j,j} + a_{i,j,i,j} + a_{i,j,j,i}) \quad (\text{A.2})$$

where δ denotes the second order tensor the components of which are δ_j^i (δ_j^i is the Kronecker symbol). No confusion should arise with the Dirac measure δ . Moreover, $::$ denotes the fourth order tensor product, defined by

$$a :: b = a_{i,j,k,l} b_{i,j,k,l},$$

for two fourth order tensors a and b .

The trace of any second order tensor \mathcal{G} is denoted by $\text{Trace } \mathcal{G}$. We recall that we note $\tilde{\nabla} = \nabla_x - \nabla_x V \partial_\varepsilon$.

We first compute the term $\mathcal{P}(L(L^{(2)}F))$, where F depends on p only through the kinetic energy $|p|^2/2$. Obviously then, $\nabla_p F = p \partial_\varepsilon F$. Then:

$$\begin{aligned} \nabla_p^{\otimes 3} F &= \nabla_p \otimes [\nabla_p \otimes (p \partial_\varepsilon F)] \\ &= \nabla_p \otimes [\delta \partial_\varepsilon F + p \otimes p \partial_\varepsilon^2 F] \\ &= (2\delta \otimes p + p \otimes \delta) \partial_\varepsilon^2 F + p^{\otimes 3} \partial_\varepsilon^3 F \end{aligned}$$

and, since $\nabla_x^{\otimes 3}V$ is a symmetric tensor, we have:

$$\begin{aligned}\nabla_x^{\otimes 3}V:\nabla_p^{\otimes 3}F &= 3\nabla_x^{\otimes 3}V:p \otimes \delta \partial_\varepsilon^2 F + \nabla_x^{\otimes 3}V:p^{\otimes 3} \partial_\varepsilon^3 F \\ &= 3p \cdot \nabla_x(\Delta V) \partial_\varepsilon^2 F + \nabla_x^{\otimes 3}V:p^{\otimes 3} \partial_\varepsilon^3 F\end{aligned}\quad (\text{A.3})$$

since $\mathcal{G} : \delta = \text{Trace}(\mathcal{G})$ for any second order tensor. Now, apply L to $\nabla_x^{\otimes 3}V:\nabla_p^{\otimes 3}F$.

First, by (A.3),

$$p \cdot \nabla_x(\nabla_x^{\otimes 3}V:\nabla_p^{\otimes 3}F) = 3p^{\otimes 2} : \nabla_x(\nabla_x(\Delta V)\partial_\varepsilon^2 F) + p^{\otimes 4} :: \nabla_x(\nabla_x^{\otimes 3}V\partial_\varepsilon^3 F) \quad (\text{A.4})$$

and, on the other hand,

$$\begin{aligned}\nabla_x V \cdot \nabla_p \left(\nabla_x^{\otimes 3}V:\nabla_p^{\otimes 3}F \right) &= 3\nabla_x V \nabla_x(\Delta V) : \nabla_p(p\partial_\varepsilon^2 F) + \nabla_x V \nabla_x^{\otimes 3}V :: \nabla_p(p^{\otimes 3}\partial_\varepsilon^3 F) \\ &= 3\nabla_x V \nabla_x(\Delta V) : (\delta\partial_\varepsilon^2 F + p^{\otimes 2}\partial_\varepsilon^3 F) \\ &\quad + \nabla_x V \nabla_x^{\otimes 3}V :: [(\delta p^{\otimes 2} + 2p^{\otimes 2}\delta)\partial_\varepsilon^3 F + p^{\otimes 4}\partial_\varepsilon^4 F].\end{aligned}\quad (\text{A.5})$$

We recall that $N(\varepsilon) = 4\pi\sqrt{2\varepsilon}$ and that, for any function $f(p)$ and any function ϕ independent of p or depending on p only through the energy $|p|^2/2$, we have $\mathcal{P}(f\phi) = \mathcal{P}(f)\phi$. Based on this, the projection on \mathcal{E} takes the form:

$$\begin{aligned}N(\varepsilon)\mathcal{P} \left(p \cdot \nabla_x(\nabla_x^{\otimes 3}V:\nabla_p^{\otimes 3}F) \right) (\varepsilon) &= N(\varepsilon)\mathcal{P} (3p^{\otimes 2}) : \nabla_x(\nabla_x(\Delta V)\partial_\varepsilon^2 F) + N(\varepsilon)\mathcal{P} (p^{\otimes 4}) :: \nabla_x(\nabla_x^{\otimes 3}V\partial_\varepsilon^3 F) \\ &= 4\pi \left\{ (2\varepsilon)^{3/2} \nabla_x \cdot (\nabla_x(\Delta V)\partial_\varepsilon^2 F) + \frac{(2\varepsilon)^{5/2}}{5} \nabla_x \cdot (\nabla_x(\Delta V)\partial_\varepsilon^3 F) \right\} \\ &= 4\pi \frac{\partial}{\partial \varepsilon} \nabla_x \cdot \left\{ \frac{(2\varepsilon)^{5/2}}{5} (\nabla_x(\Delta V)\partial_\varepsilon^2 F) \right\},\end{aligned}$$

according to (A.4) (we have used (A.1) and (A.2)). Following (A.5), we deduce

$$\begin{aligned}
& N(\varepsilon) \mathcal{P} \left(\nabla_x V \cdot \nabla_p (\nabla_x^{\otimes 3} V : \nabla_p^{\otimes 3} F) \right) (\varepsilon) \\
&= N(\varepsilon) \left\{ 3 \nabla_x V \nabla_x (\Delta V) : (\delta \partial_\varepsilon^2 F + \mathcal{P} (p^{\otimes 2}) \partial_\varepsilon^3 F) \right. \\
&\quad \left. + \nabla_x V \nabla_x^{\otimes 3} V :: [(\delta \mathcal{P} (p^{\otimes 2}) + 2 \mathcal{P} (p^{\otimes 2}) \delta) \partial_\varepsilon^3 F + \mathcal{P} (p^{\otimes 4}) \partial_\varepsilon^4 F] \right\} \\
&= 4\pi \frac{\partial}{\partial \varepsilon} \left\{ (2\varepsilon)^{3/2} \nabla_x V \cdot \nabla_x (\Delta V) \partial_\varepsilon^2 F + \frac{(2\varepsilon)^{5/2}}{5} \nabla_x V \cdot \nabla_x (\Delta V) \partial_\varepsilon^3 F \right\} \\
&= 4\pi \frac{\partial}{\partial \varepsilon} \nabla_x V \cdot \frac{\partial}{\partial \varepsilon} \left\{ \frac{(2\varepsilon)^{5/2}}{5} \nabla_x (\Delta V) \partial_\varepsilon^2 F \right\}
\end{aligned}$$

where we have used (A.1), (A.2) and the symmetries of $\nabla_x^3 V$. Therefore,

$$N(\varepsilon) \mathcal{P} (L (L^{(2)} F)) (\varepsilon) = \frac{4\pi}{24} \frac{\partial}{\partial \varepsilon} \tilde{\nabla} \cdot \left\{ \frac{(2\varepsilon)^{5/2}}{5} \nabla_x (\Delta V) \partial_\varepsilon^2 F \right\}.$$

Let us turn to $\mathcal{P}(L^{(2)}(LF))$. First, note that, for any vector $\mathcal{G}(x, \varepsilon)$ depending only on the position and the energy (such as $\tilde{\nabla} F$ and its derivatives with respect to ε), one can write

$$\nabla_p (p \cdot \mathcal{G}) = \mathcal{G} + p(p \cdot \partial_\varepsilon \mathcal{G}). \quad (\text{A.6})$$

This will be useful in the following computations. We start from $LF = p \cdot \tilde{\nabla} F$ and apply $\nabla_p^{\otimes 3}$. Using (A.6), this gives

$$\begin{aligned}
& \nabla_p^{\otimes 3} (p \cdot \tilde{\nabla} F) = \nabla_p^{\otimes 2} \left(\tilde{\nabla} F + p (p \cdot \partial_\varepsilon \tilde{\nabla} F) \right) \\
&= \nabla_p (p \partial_\varepsilon \tilde{\nabla} F) + \nabla_p (\delta (p \cdot \partial_\varepsilon \tilde{\nabla} F)) + \nabla_p (p \partial_\varepsilon \tilde{\nabla} F) + \nabla_p (p^{\otimes 2} (p \cdot \partial_\varepsilon^2 \tilde{\nabla} F)) \\
&= 3\delta \partial_\varepsilon \tilde{\nabla} F + 3p^{\otimes 2} \partial_\varepsilon^2 \tilde{\nabla} F + (2\delta p + p\delta) (p \cdot \partial_\varepsilon^2 \tilde{\nabla} F) + p^{\otimes 3} (p \cdot \partial_\varepsilon^3 \tilde{\nabla} F).
\end{aligned}$$

Using the symmetry of the third order tensor $\nabla_x^{\otimes 3} V$, we get:

$$\begin{aligned}
24L^{(2)} (LF) &= 3 \partial_\varepsilon \tilde{\nabla} F \cdot \nabla_x (\Delta V) + 3 \nabla_x^{\otimes 3} V : p^{\otimes 2} \partial_\varepsilon^2 \tilde{\nabla} F \\
&\quad + 3p^{\otimes 2} : \partial_\varepsilon^2 \tilde{\nabla} F \nabla_x (\Delta V) + p^{\otimes 4} :: \nabla_x^{\otimes 3} V \partial_\varepsilon^3 \tilde{\nabla} F.
\end{aligned}$$

Reminding (A.1) and (A.2), we have

$$\begin{aligned}
24\mathcal{P}(L^{(2)}(LF)) &= N(\varepsilon) \left(3\nabla_x(\Delta V) \cdot \partial_\varepsilon \tilde{\nabla} F \right) + 3N(\varepsilon)\mathcal{P}(p^{\otimes 2}) : \left(\partial_\varepsilon^2 \tilde{\nabla} F \nabla_x(\Delta V) \right) \\
&\quad + 3N(\varepsilon)\mathcal{P}(p^{\otimes 2}) \partial_\varepsilon^2 \tilde{\nabla} F : \nabla_x^{\otimes 3} V + N(\varepsilon)\mathcal{P}(p^{\otimes 4}) :: \partial_\varepsilon^3 \tilde{\nabla} F \nabla_x^{\otimes 3} V \\
&= 4\pi \left\{ 3(2\varepsilon)^{1/2} \nabla_x(\Delta V) \cdot \partial_\varepsilon \tilde{\nabla} F + (2\varepsilon)^{3/2} \left(2 \nabla_x(\Delta V) \cdot \partial_\varepsilon^2 \tilde{\nabla} F \right) \right. \\
&\quad \left. + \frac{(2\varepsilon)^{5/2}}{5} \left(\tilde{\nabla}(\Delta V) \cdot \partial_\varepsilon^3 \tilde{\nabla} F \right) \right\},
\end{aligned}$$

which finally gives

$$N(\varepsilon)\mathcal{P}(L^{(2)}(LF))(\varepsilon) = \frac{4\pi}{24} \frac{\partial^2}{\partial \varepsilon^2} \left\{ \frac{(2\varepsilon)^{5/2}}{5} \nabla_x(\Delta V) \cdot \partial_\varepsilon \tilde{\nabla} F \right\}.$$

B The QSHE₂ model

Let us note $\lambda = \ln F$ as in Theorem 5.2. The function λ is a function of x and ε only. We shall identify the functions $(x, p) \rightarrow \lambda(x, |p|^2/2)$ and λ when no confusion arises. We recall that, for $f(x, p) = \lambda(x, |p|^2/2)$, formula (5.8) can be rewritten as

$$\mathcal{T}\lambda(x, p) = \frac{1}{8} (\mathcal{I} + p^{\otimes 2} : \mathcal{J})$$

where \mathcal{I} and \mathcal{J} are given by (5.12) and (5.13) respectively. The expression of the trace of the second order tensor \mathcal{J} is given by (5.14).

The terms to compute are $\mathcal{P}(FT(\ln F))$ and $\mathcal{P}(L(L(FT(\ln F))))$. Since F is a function of the energy only, the first term is equal to $F\mathcal{P}(\mathcal{T}(\ln F))$.

Computation of $NF\mathcal{P}(\mathcal{T}(\ln F))$

Here, we only have to project Eq. (5.10). Using formulas (A.1) and (A.2), this equation becomes (we recall that $N(\varepsilon) = 4\pi(2\varepsilon)^{1/2}$):

$$N(\varepsilon)\mathcal{P}(\mathcal{T}\lambda) = \frac{4\pi}{8} \left(\sqrt{2\varepsilon} \mathcal{I} + \frac{(2\varepsilon)^{3/2}}{3} \text{Trace } \mathcal{J} \right)$$

where $\text{Trace } \mathcal{J}$ is explicited in (5.14).

Computation of $N\mathcal{P}(L(L(FT(\ln F))))$

We first give some expressions valid for any function G and second order tensor \mathcal{G} that depend only on the energy. It has been seen that $LG = p \cdot \tilde{\nabla}G$. Then a straightforward computation yields

$$L(LG) = L(p \cdot \tilde{\nabla}G) = p^{\otimes 2} : \tilde{\nabla}^{\otimes 2}G - \nabla_x V \cdot \tilde{\nabla}G$$

where $L(p) = -\nabla_x V$ has been used. Recalling that $N(\varepsilon) = 4\pi\sqrt{2\varepsilon}$, formula (A.1) gives

$$N(\varepsilon)\mathcal{P}(L(LG)) = 4\pi \left(\frac{(2\varepsilon)^{3/2}}{3} \tilde{\nabla} \cdot \tilde{\nabla}(G) - \sqrt{2\varepsilon} \nabla_x V \cdot \tilde{\nabla}G \right)$$

and, since $\tilde{\nabla}(2\varepsilon)^{(k+1)/2} = (k+1)(2\varepsilon)^{k/2} \nabla_x V$,

$$N(\varepsilon)\mathcal{P}(L(LG)) = 4\pi \tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{3/2}}{3} \tilde{\nabla}G \right). \quad (\text{B.1})$$

On the other hand, since L is a first order tensor, we have

$$L(L(p^{\otimes 2} : \mathcal{G})) = L(L(p^{\otimes 2})) : \mathcal{G} + 2L(p^{\otimes 2}) : L(\mathcal{G}) + p^{\otimes 2} : L(L(\mathcal{G})).$$

Obviously, $Lp = -\nabla_x V$ and $L(\nabla_x V) = p \cdot \nabla_x(\nabla_x V)$. Therefore,

$$\begin{aligned} L(L(p^{\otimes 2})) &= L(-\nabla_x V p - p \nabla_x V) \\ &= [-p \cdot \nabla_x(\nabla_x V)]p - p[p \cdot \nabla_x(\nabla_x V)] + 2\nabla_x V \nabla_x V. \end{aligned} \quad (\text{B.2})$$

Since \mathcal{G} depends only on the energy, we have $L\mathcal{G} = p \cdot \tilde{\nabla}(\mathcal{G})$ and, consequently,

$$L(L(\mathcal{G})) = (p^{\otimes 2} : \tilde{\nabla}^{\otimes 2})\mathcal{G} - \nabla_x V \cdot \tilde{\nabla}(\mathcal{G}). \quad (\text{B.3})$$

Therefore, reminding that $L(p) = -\nabla_x V$, $L\mathcal{G} = p \cdot \tilde{\nabla}(\mathcal{G})$, that \mathcal{G} is symmetric, and using (B.2) and (B.3), we obtain

$$\begin{aligned} L(L(p^{\otimes 2} : \mathcal{G})) &= [-(2p \cdot \nabla_x(\nabla_x V))p + 2\nabla_x V \nabla_x V] : \mathcal{G} \\ &\quad + 4(-\nabla_x V)p : p \cdot \tilde{\nabla}(\mathcal{G}) + p^{\otimes 4} :: \tilde{\nabla}^{\otimes 2}\mathcal{G} - p^{\otimes 2} : \nabla_x V \cdot \tilde{\nabla}(\mathcal{G}), \end{aligned}$$

which, according to (A.1) and (A.2), yields

$$\begin{aligned}
N(\varepsilon)\mathcal{P} [L(L(p^{\otimes 2} : \mathcal{G}))] &= 4\pi \left\{ 2 \left(-\frac{(2\varepsilon)^{3/2}}{3} \nabla_x^{\otimes 2} V + \sqrt{2\varepsilon} \nabla_x V \nabla_x V \right) : \mathcal{G} \right. \\
&+ 4 \frac{(2\varepsilon)^{3/2}}{3} \left(-\nabla_x V \tilde{\nabla} \right) : \mathcal{G} + \frac{(2\varepsilon)^{5/2}}{15} \left(\tilde{\nabla} \cdot \tilde{\nabla} (\text{Trace } \mathcal{G}) + 2 \tilde{\nabla}^{\otimes 2} : \mathcal{G} \right) \\
&\left. - \frac{(2\varepsilon)^{3/2}}{3} \nabla_x V \cdot \tilde{\nabla} (\text{Trace } \mathcal{G}) \right\}
\end{aligned}$$

Finally, using again $\tilde{\nabla} (2\varepsilon)^{(k+1)/2} = (k+1) (2\varepsilon)^{k/2} \nabla_x V$, we have

$$N(\varepsilon)\mathcal{P} [L(L(p^{\otimes 2} : \mathcal{G}))] = 4\pi \left\{ 2\tilde{\nabla}^{\otimes 2} : \frac{(2\varepsilon)^{5/2}}{15} \mathcal{G} + \tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{5/2}}{3} \tilde{\nabla} \text{Trace } \mathcal{G} \right) \right\}. \tag{B.4}$$

Let us go back to the computation of $N\mathcal{P}(L(L(FT(\ln F))))$. Taking for G the function $F\mathcal{I}$ and, for \mathcal{G} , the second order tensor $F\mathcal{J}$, Equations (B.1) and (B.4) allow to conclude that

$$\begin{aligned}
N\mathcal{P}(L(L(FT(\ln F)))) &= \frac{4\pi}{8} \left\{ \tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{3/2}}{3} \tilde{\nabla} (F\mathcal{I}) \right) + 2\tilde{\nabla}^{\otimes 2} : \frac{(2\varepsilon)^{5/2}}{15} (F\mathcal{J}) \right. \\
&\left. + \tilde{\nabla} \cdot \left(\frac{(2\varepsilon)^{5/2}}{3} \tilde{\nabla} (F \text{Trace } \mathcal{J}) \right) \right\},
\end{aligned}$$

since by (5.11) we have $FT(\ln F) = F\mathcal{I} + p^{\otimes 2} : F\mathcal{J}$.

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