

QUANTUM DRIFT-DIFFUSION MODELING OF SPIN TRANSPORT IN NANOSTRUCTURES

LUIGI BARLETTI AND FLORIAN MÉHATS

ABSTRACT. We consider a two-dimensional electron gas with a spin-orbit interaction of Bychkov and Rashba type. Starting from a microscopic model, represented by the von Neumann equation endowed with a suitable BGK collision term, we apply the Chapman-Enskog method to derive a quantum diffusive model. Such model is then semiclassically expanded up to second order, leading to nonlinear quantum corrections to the zero-order diffusive models of the literature.

1. INTRODUCTION

In this article, we derive models describing at a diffusive scale the quantum transport of a spin-polarized bidimensional electron gas, including a description of spin-orbit interactions. The target applications are spintronic devices, which involve the active control and manipulation of spin degrees of freedom in solid-states systems, see Ref. [30] for a comprehensive review on this subject, including a discussion of spin relaxation mechanisms. Semiclassical drift-diffusion models for spin systems [24, 26, 28] offer a reasonable numerical cost, but are not designed to take into account quantum effects. In Refs. [5] and [16], a hierarchy of diffusion models for spin transport is derived by applying a diffusion asymptotics to the semiclassical Boltzmann equation. We present here a strategy based on an entropy minimization technique in order to derive quantum corrections to drift-diffusion models for spins. To this end, we follow the programme of Refs. [10] and [14]: we first identify a ballistic transport system, then include a description of collisions in this transport picture and derive a macroscopic approximation of the so-obtained kinetic quantum system.

Modeling collision mechanisms in a fully quantum mechanical setting is a complicated matter (see Refs. [2, 3, 7, 18] for an overview). However, since the final result is a model for the evolution of macroscopic quantities (typically, the density), the main information about the microscopic collision mechanism entering the macroscopic model is the form of the local equilibrium, i.e. of the integral invariants of the collisions. The main ingredient of our strategy is the definition of a quantum generalization of Maxwellian as the minimizer of the free energy under a density constraint. This will enable to define a caricature of collision operator, chosen as a simple BGK operator relaxing towards this local equilibrium.

Since the bidimensional electron gas is spin-polarized, two species of particles are taken into account from the beginning in our description. Hence,

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the microscopic model from which we start the analysis will be the quantum Liouville (or von Neumann) equation for density operators under the form of 2×2 matrices of operators. Note that the Hamiltonian will not be diagonal because of the spin-orbit interactions. Therefore, the quantum Maxwellian in our case will also take the form of 2×2 non diagonal matrices, and the final model will display a vectorial structure with coupling terms. Deriving a quantum drift-diffusion with vectorial structure is the main contribution of this paper, compared to the previous works deriving entropic quantum macroscopic models: quantum drift-diffusion, energy transport or SHE models [6, 14, 15] or quantum hydrodynamics [12, 13, 21, 22]. For an overview of macroscopic quantum models, one can refer to the recent book Ref. [20]. Note that, recently, two other vectorial quantum drift-diffusion have been derived: in Ref. [25] the case of subband systems was studied and, in Ref. [4], the diffusive limit of the two band k-p model was investigated. The numerical validation of our approach will be investigated in a future work and should be done following the strategy settled in the scalar case in Refs. [11], [19].

This paper is divided into two parts. In Section 2, we present our main results and Section 3 is devoted to the proofs.

2. MAIN RESULTS

In this section, we present our main results. First, in Subsection 2.1, we introduce the microscopic quantum transport model. Then, in Subsection 2.2, we define the local quantum equilibrium by entropy minimization and define the associated BGK operator. Finally, in Subsection 2.3, we give the macroscopic limit of the quantum BGK system: the quantum drift-diffusion model, which dissipates the fluid quantum entropy. We also perform formally the semiclassical limit for this system, which gives the classical drift-diffusion model for spin systems, and we provide the next order approximation, which is a drift-diffusion model with Bohm potentials.

2.1. Microscopic model and scaling. A two dimensional electron gas (2DEG) in the (x, y) -plane with a Bychkov-Rashba spin-orbit interaction can be described by means of the following Hamiltonian:

$$H = \left(-\frac{\hbar^2}{2m} \Delta + eV \right) I - \hbar \alpha_{so} \begin{pmatrix} 0 & i\partial_y - \partial_x \\ i\partial_y + \partial_x & 0 \end{pmatrix}. \quad (1)$$

Here, I is the 2×2 identity matrix, m is the electron effective mass, e is the (positive) elementary charge and α_{so} is the Rashba constant [8, 30]. The electric potential V may be either assigned or self-consistently determined by a Poisson equation. In this paper, for simplicity, we shall consider the potential as given. Since the system is 2-dimensional, throughout this paper we shall use the notations

$$\mathbf{x} = (x, y), \quad \mathbf{p} = (p_x, p_y)$$

to denote, respectively, the position and momentum coordinates.

If ϱ denotes the density operator of the system, the evolution equation for $\varrho = \varrho(t)$ in absence of collision, is the von Neumann equation

$$i\hbar \partial_t \varrho(t) = [H, \varrho(t)].$$

In order to take account of collisional processes in a relatively simple way, we add a BGK-like term:

$$i\hbar \partial_t \varrho(t) = [H, \varrho(t)] + i\hbar Q(\varrho(t)), \quad (2)$$

where

$$Q(\varrho(t)) = \frac{1}{\tau_p} (\varrho_{eq}(t) - \varrho(t)). \quad (3)$$

The BGK collision operator Q is assumed to conserve electron spin and density and to relax momentum with relaxation time τ_p . The local equilibrium state $\varrho_{eq}(t)$ depends non-linearly and non-locally on $\varrho(t)$ and will be discussed in detail in the next section.

In order to re-write the von Neumann-BGK equation (2) in dimensionless form, let us introduce the reference length L , time t_0 , potential V_0 and density N , and consider the dimensionless quantities

$$\tilde{x} = x/L, \quad \tilde{y} = y/L, \quad \tilde{t} = t/t_0, \quad \tilde{V} = V/V_0, \quad \tilde{\varrho} = \varrho/N.$$

For such quantities, Eq. (2) becomes

$$\frac{i\hbar N}{t_0} \partial_{\tilde{t}} \tilde{\varrho}(\tilde{t}) = [\tilde{H}, N \tilde{\varrho}(\tilde{t})] + \frac{i\hbar N}{\tau_p} (\tilde{\varrho}_{eq}(\tilde{t}) - \tilde{\varrho}(\tilde{t})),$$

where

$$\tilde{H} = \left(-\frac{\hbar^2}{2mL^2} \Delta + eV_0 \tilde{V} \right) I - \frac{\hbar \alpha_{so}}{L} \begin{pmatrix} 0 & i\partial_{\tilde{y}} - \partial_{\tilde{x}} \\ i\partial_{\tilde{y}} + \partial_{\tilde{x}} & 0 \end{pmatrix}.$$

From now on we shall switch definitively to the adimensional quantities and so, in order to lighten the notations, we shall drop the tildes. If we divide both sides by N and by the reference energy p_0^2/m , where

$$p_0 = \sqrt{mk_0 T},$$

(k_0 is Boltzmann's constant and T is the temperature), we finally obtain the adimensional form of the von Neumann-BGK equation (2):

$$i\tau \varepsilon \partial_t \varrho(t) = [H_\varepsilon, \varrho(t)] + \frac{i\varepsilon}{\tau} (\varrho_{eq}(t) - \varrho(t)), \quad (4)$$

where

$$H_\varepsilon = \left(-\frac{\varepsilon^2}{2} \Delta + \phi \right) I - \varepsilon^2 \alpha \begin{pmatrix} 0 & i\partial_y - \partial_x \\ i\partial_y + \partial_x & 0 \end{pmatrix} \quad (5)$$

and

$$\begin{aligned} \varepsilon &= \frac{\hbar}{p_0 L} = \frac{\hbar}{\sqrt{mk_0 T L^2}}, & \tau &= \frac{p_0 \tau_p}{mL} = \tau_p \sqrt{\frac{k_0 T}{mL^2}}, \\ \alpha &= \frac{mL \alpha_{so}}{\hbar}, & \phi(\mathbf{x}) &= \frac{meV_0}{p_0^2} V(\mathbf{x}). \end{aligned} \quad (6)$$

Note that ε is a semiclassical parameter, τ is a diffusive parameter (the scaled mean collisional time), and α is the scaled Rashba constant. Moreover, the time scale has been chosen equal to $\frac{m^2 L}{\tau_p p_0}$. In Table 2.1 we report the typical values of some dimensional and adimensional parameters for the 2DEGs arising in two different semiconductor heterostructures (characterized by particularly large Rashba constants). The first one (HS1) is a GaN/AlGaN/GaN heterostructure, as reported by Ref. [27]. The second one (HS2) is a InAlAs/InGaAs/InAlAs asymmetric quantum well, as reported

	m	$\hbar\alpha_{so}$	ε	τ	α
HS1	$0.2 m_e$	$6 \times 10^{-13} \text{ eV} \cdot \text{m}$	7.2×10^{-2}	7.7×10^{-2}	1.7×10^{-1}
HS2	$0.04 m_e$	$1 \times 10^{-12} \text{ eV} \cdot \text{m}$	1.7×10^{-2}	1.6×10^{-2}	5.7×10^{-2}

TABLE 1. Values of some parameters for 2DEGs in two different experimental spintronic devices. HS1 is a GaN/AlGa_N/GaN heterostructure, for which the values are taken from Ref. [27]. HS2 is a InAlAs/InGaAs/InAlAs asymmetric quantum well, for which the values are taken from Ref. [23]. In both cases we have chosen $L = 10^{-7} \text{ m}$, $T = 77 \text{ K}$, and $\tau_p = 10^{-13} \text{ s}$. m_e is the electron bare mass.

by Ref. [23]. In both cases we have chosen as reference values $L = 100 \text{ nm}$, $T = 77 \text{ K}$, and $\tau_p = 10^{-13} \text{ s}$. The strength of the adimensionalized external field ϕ depends on the assumption about the operating regime of the device. If the field range is between 10^{-2} V and 10^{-1} V , then ϕ is between 1 and 10. It turns out that in these two typical cases, the three parameters ε , τ and α are small compared to unity. Since our objective is to obtain a quantum model at the diffusive scale, in a first step we shall perform the limit $\tau \rightarrow 0$ with ε and α fixed. Then, in a second step, we shall discuss the approximations of such diffusive model for small ε and α , obtaining a semiclassical model with quantum corrections.

2.2. Definition of the local equilibrium by entropy minimization.

Let us now discuss the local equilibrium density-operator $\varrho_{eq}(t)$ appearing in Eq. (4). We shall follow the approach of Degond and Ringhofer [10, 14] which consists in defining $\varrho_{eq}(t)$ as the minimizer of a suitable quantum entropy functional under the constraint that $\varrho_{eq}(t)$ and $\varrho(t)$ share certain local moments. Such moments, therefore, are conserved by the BGK collision operator Q and, moreover, closed equations for such moments can be derived.

To this aim, we first need a notion for local moments (see Ref. [10]). Let ϱ be a scalar (no spin) density operator. The local density $n(\mathbf{x})$ associated to ϱ can be defined by duality as follows

$$\text{Tr} \{ \varphi \varrho \} = \int_{\mathbb{R}^2} \varphi(\mathbf{x}) n(\mathbf{x}) d\mathbf{x}, \quad \forall \varphi \in C_0^\infty(\mathbb{R}^2). \quad (7)$$

Note that φ is a test function and has to be considered as a multiplication operator in the left-hand side of (7). This definition is the rigorous version of the intuitive definition (not suitable in a L^2 theory)

$$n(\mathbf{x}) = \varrho(\mathbf{x}, \mathbf{x}),$$

where $\varrho(\mathbf{x}, \mathbf{x}')$ is the density matrix, i.e. the kernel of the density operator ϱ . By introducing the Wigner function [29]

$$w(\mathbf{x}, \mathbf{p}) = \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^2} \varrho \left(\mathbf{x} + \frac{\boldsymbol{\xi}}{2}, \mathbf{x} - \frac{\boldsymbol{\xi}}{2} \right) e^{-i\boldsymbol{\xi} \cdot \mathbf{p}/\hbar} d\boldsymbol{\xi}, \quad (8)$$

the above definition can also be written in a quasi-classical fashion:

$$n(\mathbf{x}) = \int_{\mathbb{R}^2} w(\mathbf{x}, \mathbf{p}) d\mathbf{p}. \quad (9)$$

In the same spirit, it is natural to define the local density of current $\mathbf{J} = (J_x, J_y)$ associated to ϱ by means of the duality relation

$$\mathrm{Tr} \left\{ \left(\varphi \cdot \nabla + \frac{1}{2} \mathrm{div} \varphi \right) \varrho \right\} = \frac{i}{\varepsilon} \int_{\mathbb{R}^2} \varphi(\mathbf{x}) \cdot \mathbf{J}(\mathbf{x}) d\mathbf{x}, \quad \forall \varphi \in [C_0^\infty(\mathbb{R}^2)]^2 \quad (10)$$

or, by means of the Wigner function,

$$\mathbf{J}(\mathbf{x}) = \int_{\mathbb{R}^2} \mathbf{p} w(\mathbf{x}, \mathbf{p}) d\mathbf{p} \quad (11)$$

and both definitions are formally equivalent to the intuitive definition from quantum mechanics textbooks:

$$\mathbf{J}(\mathbf{x}) = -\frac{i\varepsilon}{2} (\nabla_{\mathbf{x}} - \nabla_{\mathbf{x}'}) \varrho(\mathbf{x}, \mathbf{x}', t) |_{\mathbf{x}=\mathbf{x}'}$$

In the spinorial case, all these quantities take also the spin indices. Thus, for example, n_{ij} , $\mathbf{J}^{ij} = (J_x^{ij}, J_y^{ij})$ will be the local densities associated to the ij -component ϱ_{ij} of ϱ .

Coming back to our local equilibrium, we assume that collisions conserve the number of electrons and their spins (the spin relaxation mechanism is assumed to pertain to the spin-orbit coupling). Thus, the BGK operator should conserve the spin-up and spin-down electron densities

$$n_1 \equiv n_{11} \quad \text{and} \quad n_2 \equiv n_{22}$$

which, according to the above discussion, are defined either by

$$\mathrm{Tr} \left\{ \varrho \begin{pmatrix} \varphi_1 & 0 \\ 0 & \varphi_2 \end{pmatrix} \right\} = \int_{\mathbb{R}^2} \varphi_1(\mathbf{x}) n_1(\mathbf{x}) + \varphi_2(\mathbf{x}) n_2(\mathbf{x}) d\mathbf{x}, \quad \forall \varphi_1, \varphi_2 \in C_0^\infty(\mathbb{R}^2). \quad (12)$$

or by

$$n_1(\mathbf{x}) = \int_{\mathbb{R}^2} w_{11}(\mathbf{x}, \mathbf{p}) d\mathbf{p}, \quad n_2(\mathbf{x}) = \int_{\mathbb{R}^2} w_{22}(\mathbf{x}, \mathbf{p}) d\mathbf{p}. \quad (13)$$

We introduce the operators \mathcal{N}_1 and \mathcal{N}_2 that act on the density matrix ϱ taking the two associated moments n_1 and n_2 , i.e.

$$(\mathcal{N}_1 \varrho)(\mathbf{x}) := n_1(\mathbf{x}), \quad (\mathcal{N}_2 \varrho)(\mathbf{x}) := n_2(\mathbf{x}).$$

Let us assume that the system is in thermal equilibrium with a bath at a given temperature T . Then, the convenient entropy functional to be used in this case [14] is the quantum free energy

$$G(\varrho) = \mathrm{Tr} \left\{ k_0 T \varrho \left(\ln \frac{\varrho}{N} - I \right) + H \varrho \right\}, \quad (14)$$

which in adimensional form (keeping the same notation for adimensional quantities) reads as follows

$$G(\varrho) = \mathrm{Tr} \{ \varrho (\ln \varrho - I) + H_\varepsilon \varrho \}. \quad (15)$$

Adapting to the present case the theory of Degond and Ringhofer [10], we can choose the local equilibrium $\varrho_{eq}(t)$, appearing in the BGK operator (3),

as the minimizer of G which has the same moments (n_1, n_2) as $\varrho(t)$. To this aim, we give the following definitions.

Definition 1. *Let the functions n_1 and n_2 be given. Consider the following constrained minimization problem:*

$$\min \{ G(\varrho) \mid \varrho \text{ is a density operator satisfying } \mathcal{N}_1 \varrho = n_1 \text{ and } \mathcal{N}_2 \varrho = n_2 \}. \quad (16)$$

The solution of such problem, if it exists, is called the local equilibrium density operator (“quantum Maxwellian”) associated to n_1 and n_2 and will be denoted by $M_{n_1 n_2}$. The BGK local equilibrium state ϱ_{eq} appearing in (3) is defined as

$$\varrho_{eq}(t) = M_{\mathcal{N}_1 \varrho(t) \mathcal{N}_2 \varrho(t)} \quad (17)$$

and is, therefore, the minimum-entropy state which has the same spin densities as $\varrho(t)$.

A necessary condition [14, 10] on $M_{n_1 n_2}$ is that two scalar real-valued functions $A_1 = A_1(n_1, n_2)$ and $A_2 = A_2(n_1, n_2)$ – the Lagrange multipliers associated to the two constraints – exist such that

$$M_{n_1 n_2} = \exp(-H_\varepsilon^A), \quad (18)$$

where H_ε^A is the modified Hamiltonian

$$H_\varepsilon^A = H_\varepsilon + \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix} = \begin{pmatrix} -\frac{\varepsilon^2}{2} \Delta + \phi + A_1 & \varepsilon^2 \alpha(\partial_x - i\partial_y) \\ -\varepsilon^2 \alpha(\partial_x + i\partial_y) & -\frac{\varepsilon^2}{2} \Delta + \phi + A_2 \end{pmatrix} \quad (19)$$

The functions A_1 and A_2 are called chemical potentials and have a functional dependence on n_1 and n_2 resulting from the constraints $\mathcal{N}_i M_{n_1 n_2} = n_i$, i.e.

$$\mathcal{N}_1 \exp(-H_\varepsilon^A) = n_1, \quad \mathcal{N}_2 \exp(-H_\varepsilon^A) = n_2. \quad (20)$$

Let us summarize (17)–(20) by saying that ϱ_{eq} is characterized by

$$\begin{cases} \varrho_{eq} = \exp(-H_\varepsilon^A), \\ \mathcal{N}_{1,2} \varrho_{eq}(t) = n_{1,2}(t) = \mathcal{N}_{1,2} \varrho(t). \end{cases} \quad (21)$$

With such a definition of ϱ_{eq} , the BGK operator Q (definition (3)) has the following formal properties, mandatory in order to define a physical quantum dynamics (see Ref. [1] where quantum Liouville equations with relaxation operators are studied):

- (i) Q locally conserves the moments $n_{1,2}$, i.e.,

$$[\mathcal{N}_{1,2} Q(\varrho)](\mathbf{x}) = 0;$$

- (ii) Q dissipates the quantum entropy, i.e.,

$$\mathrm{Tr}\{Q(\varrho)G'(\varrho)\} \leq 0,$$

where $G'(\varrho) = \ln \varrho + H_\varepsilon$;

- (iii) Q preserves the positivity of operators, i.e., the formal solution of (4) with $\varrho(t=0) \geq 0$ satisfies $\varrho(t) \geq 0$ for all $t \geq 0$;

The proofs of these properties can be straightforwardly adapted from Refs. [10] and [14].

2.3. Drift-diffusion models. In Section 3.1 we shall formally prove the following theorem about the quantum ($\varepsilon \sim 1$, $\alpha \sim 1$) diffusive ($\tau \rightarrow 0$) limit of the von Neumann-BGK equation (4).

Theorem 1 (Formal diffusive limit). *Let $\varrho(t) = \varrho^\tau(t)$ be the solution of Eq. (4). Then, as $\tau \rightarrow 0$, we have $\varrho^\tau \rightarrow \varrho_0$, where ϱ_0 is the "quantum Maxwellian"*

$$\varrho_0 = M_{n_1 n_2} = \exp(-H_\varepsilon^A), \quad A_{1,2} = A_{1,2}(n_1, n_2),$$

where H_ε^A is defined by (19), and the spin densities n_1, n_2 are solutions of

$$\begin{aligned} \partial_t n_1 + \operatorname{div}(n_1 \nabla A_1) + \alpha(A_1 - A_2) \operatorname{Re}(\mathcal{D}n_{21}) - 2\alpha \operatorname{Re}(n_{21} \mathcal{D}A_2) \\ - \frac{2\alpha}{\varepsilon}(A_1 - A_2) \operatorname{Im}(J_x^{21} - iJ_y^{21}) = 0 \\ \partial_t n_2 + \operatorname{div}(n_2 \nabla A_2) + \alpha(A_1 - A_2) \operatorname{Re}(\mathcal{D}n_{21}) + 2\alpha \operatorname{Re}(n_{21} \mathcal{D}A_1) \\ + \frac{2\alpha}{\varepsilon}(A_1 - A_2) \operatorname{Im}(J_x^{21} - iJ_y^{21}) = 0. \end{aligned} \quad (22)$$

In Eq. (22) $\mathcal{D} = \partial_x - i\partial_y$, $\mathbf{J}^{ij} = (J_x^{ij}, J_y^{ij})$ is the current associated to ϱ_0 and n_{21} is the off-diagonal term of the density (see definitions (9) and (10) with spin indices).

We stress once again the fact that the chemical potentials $A_{1,2}$ (and, therefore, the current term $J_x^{21} - iJ_y^{21}$ and the off-diagonal density n_{21}) depend on the spin densities $n_{1,2}$ through the inversion of the relation (20).

In terms of the total density n and spin-polarization n_s , defined by

$$n = n_1 + n_2, \quad n_s = n_1 - n_2, \quad (23)$$

the previous system can also be written as follows:

$$\begin{aligned} \partial_t n + \operatorname{div}(n_1 \nabla A_1 + n_2 \nabla A_2) + 2\alpha \operatorname{Re} \{ \mathcal{D} [n_{21} (A_1 - A_2)] \} = 0 \\ \partial_t n_s + \operatorname{div}(n_1 \nabla A_1 - n_2 \nabla A_2) - 2\alpha \operatorname{Re} \{ n_{21} \mathcal{D} (A_1 + A_2) \} \\ - \frac{4\alpha}{\varepsilon} (A_1 - A_2) \operatorname{Im}(J_x^{21} - iJ_y^{21}) = 0. \end{aligned} \quad (24)$$

This theorem is formally proved in Subsection 3.1. System (22) (or, equivalently, (24)), together with Eq. (20), represents a fully quantum "drift diffusion" model of spin transport of electrons subject to Rashba spin-orbit interaction. An important property of this system, which is a straightforward consequence of the dissipative properties of the BGK operator Q , is the fact that it satisfies an entropy dissipation property. The following lemma is stated without proof and is directly adapted from Ref. [14].

Lemma 1. *Define the quantum fluid entropy of the system by*

$$\mathcal{S}(n_1, n_2) = \operatorname{Tr} \{ \varrho_0 (\ln \varrho_0 - I) + H_\varepsilon \varrho_0 \}, \quad \text{with } \varrho_0 = M_{n_1, n_2}.$$

Then the solution n_1, n_2 of (22) satisfies

$$\frac{d}{dt} \mathcal{S}(n_1, n_2) \leq \int (n_1 + n_2) \partial_t \phi \, dx.$$

If the potential ϕ is independent of time, then \mathcal{S} is not-increasing in time.

The practical utility of the quantum drift-diffusion model for numerical simulations may be rather limited by the difficult step of inverting the relation (20). Indeed, as we already noticed, the local equilibrium operator $\exp(-H_\varepsilon^A)$ has a complicated, functional, dependence on the chemical potentials $A_{1,2}$, which is difficult to explicit unless suitable approximations are used. However, system (22) (and the relation (20) itself) contains two other parameters which are small in most applications, that are the semiclassical parameter ε and the scaled Rashba constant α . Thus, our next step consists in expanding semiclassically the quantum model (22)+(20) in order to obtain more treatable semiclassical drift-diffusion models. This will be done up to order $\varepsilon^2 + \alpha^2$. More precisely, in Sec. 3.2, we shall compute some terms of the expansion of the local equilibrium

$$\varrho_{eq} = \varrho_{eq}^{(0)} + \varepsilon \varrho_{eq}^{(1)} + \varepsilon^2 \varrho_{eq}^{(2)} + \dots$$

and the corresponding (approximated) explicit expressions of $A_{1,2}$ and $J_x^{21} - iJ_y^{21}$ as functions of n_1 and n_2 . Note that, because of the factor $1/\varepsilon$ in some terms of Eq. (22), in order to get a diffusive model of order 2, we need to compute the above expansion up to order 3. The result of our analysis is the following drift-diffusion system with quantum corrections.

Theorem 2 (Formal semiclassical approximation). *Let $n_1^{\varepsilon,\alpha}, n_2^{\varepsilon,\alpha}$ the solution of the quantum drift-diffusion model (22). Then we formally have*

$$n_i^{\varepsilon,\alpha} = n_i + \mathcal{O}(\varepsilon^2\alpha^2), \quad i = 1, 2$$

as $\varepsilon \rightarrow 0$ and $\alpha \rightarrow 0$, where n_1, n_2 satisfy the following system:

$$\begin{aligned} \partial_t n_1 - \operatorname{div}(\nabla n_1 + n_1 \nabla \phi) + \varepsilon^2 \operatorname{div}[n_1 \nabla Q(n_1)] &= 4\alpha^2(n_2 - n_1), \\ \partial_t n_2 - \operatorname{div}(\nabla n_2 + n_2 \nabla \phi) + \varepsilon^2 \operatorname{div}[n_2 \nabla Q(n_2)] &= 4\alpha^2(n_1 - n_2), \end{aligned} \quad (25)$$

and where

$$Q(n_i) = \frac{1}{6} \frac{\Delta \sqrt{n_i}}{\sqrt{n_i}} \quad (26)$$

is the well-known Bohm potential.

Note that, at order 0 in ε , we obtain a linear system of two drift-diffusion equations with a simple coupling term, $4\alpha^2(n_i - n_j)$, which is the well known D'yakonov-Perel' spin-relaxation mechanism [30], here derived from "first principles". Note that a similar model was derived in Ref. [16] from the semiclassical Boltzmann equation by a diffusion scaling. Next, we have a correction of order ε^2 which takes the form of a Bohm potential term for each spin population.

This theorem is proved in Subsection 3.3. This proof consists in an expansion of the quantum drift-diffusion system (22) with respect to the semiclassical parameter $\varepsilon \rightarrow 0$ only (the parameter α being considered as fixed). We shall prove in fact that this semiclassical expansion leads to

$$n_i^{\varepsilon,\alpha} = \tilde{n}_i + \mathcal{O}(\varepsilon^4), \quad i = 1, 2$$

as $\varepsilon \rightarrow 0$, where \tilde{n}_1, \tilde{n}_2 satisfy the following system:

$$\begin{aligned} \partial_t \tilde{n}_1 - \operatorname{div}(\nabla \tilde{n}_1 + \tilde{n}_1 \nabla \phi) + \varepsilon^2 \operatorname{div}[\tilde{n}_1 \nabla Q(\tilde{n}_1)] \\ = 4\alpha^2(\tilde{n}_2 - \tilde{n}_1) + \varepsilon^2 \alpha^2 C_1(\tilde{n}_1, \tilde{n}_2) + \varepsilon^2 \alpha^4 C_2(\tilde{n}_1, \tilde{n}_2), \\ \partial_t \tilde{n}_2 - \operatorname{div}(\nabla \tilde{n}_2 + \tilde{n}_2 \nabla \phi) + \varepsilon^2 \operatorname{div}[\tilde{n}_2 \nabla Q(\tilde{n}_2)] \\ = 4\alpha^2(\tilde{n}_1 - \tilde{n}_2) + \varepsilon^2 \alpha^2 C_1(\tilde{n}_2, \tilde{n}_1) + \varepsilon^2 \alpha^4 C_2(\tilde{n}_2, \tilde{n}_1). \end{aligned} \quad (27)$$

In this system, C_1 and C_2 are second-order, non-linear coupling terms to be described later in more details (see Eqs. (75) and (76)). Theorem 2 can be simply deduced from this result by remarking that the constants $\varepsilon^2 \alpha^2$ and $\varepsilon^2 \alpha^4$ multiplying C_1 and C_2 are small compared to ε^2 and α^2 . Hence we obtain (25) by dropping the corresponding terms in (27).

3. PROOFS OF THE MAIN RESULTS

3.1. Chapman-Enskog expansion. In this section we study the behaviour of the von Neumann-BGK equation (4) in the diffusive limit $\tau \rightarrow 0$, we prove Theorem 1 and deduce the quantum drift-diffusion equations (22). The main tool will be the Chapman-Enskog method [9].

As in the previous section, let A_1, A_2 be the chemical potentials, let

$$\mathcal{D} = \partial_x - i\partial_y \quad (28)$$

and let φ_1, φ_2 be two test functions. Let us define the operators

$$\mathbb{A} = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}, \quad \mathbb{B} = \begin{pmatrix} 0 & \mathcal{D} \\ \mathcal{D}^* & 0 \end{pmatrix}, \quad \Phi = \begin{pmatrix} \varphi_1 & 0 \\ 0 & \varphi_2 \end{pmatrix}, \quad (29)$$

where, of course, $\mathcal{D}^* = -\partial_x - i\partial_y$. Then, recalling (5) and (19), we write

$$H_\varepsilon = -\frac{\varepsilon^2}{2} \Delta I + \phi I + \varepsilon^2 \alpha \mathbb{B} \quad (30)$$

and

$$H_\varepsilon^A = H_\varepsilon + \mathbb{A}. \quad (31)$$

Multiplying (4) by τ , it comes that, formally, the solution ϱ^τ of this equation is such that

$$\varrho^\tau = \varrho_{eq} + \mathcal{O}(\tau), \quad \text{where we have denoted } \varrho_{eq} = M_{\mathcal{N}_1 \varrho^\tau, \mathcal{N}_2 \varrho^\tau}. \quad (32)$$

Assuming that $n_1^\tau = \mathcal{N}_1 \varrho^\tau$ and $n_2^\tau = \mathcal{N}_2 \varrho^\tau$ converge to some macroscopic densities n_1 and n_2 as $\tau \rightarrow 0$, our aim is to express a time evolution system satisfied by this limit (n_1, n_2) .

Since the mapping $(n_1, n_2) \mapsto M_{n_1, n_2}$ is assumed to be continuous, we already deduce from (32) that

$$\varrho^\tau \rightarrow \varrho_0 := M_{n_1, n_2} \quad \text{as } \tau \rightarrow 0. \quad (33)$$

This formally proves the first statement of Theorem 1. The Chapman-Enskog consists now in introducing ϱ_1 , the perturbation of the local quantum Maxwellian defined according to

$$\varrho^\tau = \varrho_{eq} + \tau \varrho_1, \quad \text{where } \varrho_{eq} = M_{n_1^\tau, n_2^\tau}. \quad (34)$$

Inserting this Ansatz into (4) yields

$$i\tau \varepsilon \partial_t \varrho^\tau = [H_\varepsilon, \varrho_{eq}] + \tau [H_\varepsilon, \varrho_1] - i\varepsilon \varrho_1. \quad (35)$$

Hence,

$$\begin{aligned} i\varepsilon \varrho_1 &= [H_\varepsilon, \varrho_{eq}] + \tau[H_\varepsilon, \varrho_1] - i\tau\varepsilon \partial_t \varrho^\tau \\ &= [H_\varepsilon + \mathbb{A}, \varrho_{eq}] - [\mathbb{A}, \varrho_{eq}] + \tau[H_\varepsilon, \varrho_1] - i\tau\varepsilon \partial_t \varrho^\tau \\ &= -[\mathbb{A}, \varrho_{eq}] + \tau[H_\varepsilon, \varrho_1] - i\tau\varepsilon \partial_t \varrho^\tau, \end{aligned}$$

since ϱ_{eq} clearly commutes with $H_\varepsilon + \mathbb{A}$. This gives

$$\varrho_1 = \frac{i}{\varepsilon} [\mathbb{A}, \varrho_{eq}] + \mathcal{O}(\tau). \quad (36)$$

Substituting this expression for ϱ_1 in (35), we get

$$i\tau\varepsilon \partial_t \varrho^\tau = -[\mathbb{A}, \varrho_{eq}] + \frac{i\tau}{\varepsilon} [H_\varepsilon, [\mathbb{A}, \varrho_{eq}]] + \frac{i\varepsilon}{\tau} (\varrho_{eq} - \varrho^\tau) + \mathcal{O}(\tau^2). \quad (37)$$

Let us now apply the moments operators \mathcal{N}_1 and \mathcal{N}_2 to this equation. Using that, by construction, $\mathcal{N}_{1,2}(\varrho_{eq} - \varrho^\tau) = 0$ (see Definition 1), we get

$$\partial_t n_{1,2}^\tau = \frac{i}{\tau\varepsilon} \mathcal{N}_{1,2}[\mathbb{A}, \varrho_{eq}] + \frac{1}{\varepsilon^2} \mathcal{N}_{1,2}[H_\varepsilon, [\mathbb{A}, \varrho_{eq}]] + \mathcal{O}(\tau), \quad (38)$$

that is,

$$\text{Tr} \{ \partial_t \varrho^\tau \Phi \} = \frac{i}{\tau\varepsilon} \text{Tr} \{ [\mathbb{A}, \varrho_{eq}], \Phi \} + \frac{1}{\varepsilon^2} \text{Tr} \{ [H_\varepsilon, [\mathbb{A}, \varrho_{eq}], \Phi \} + \mathcal{O}(\tau), \quad (39)$$

for any couple of test functions φ_1 and φ_2 (see definitions (12) and (29)). Now we claim the following crucial property, mandatory to pass to the limit as $\tau \rightarrow 0$ in (39). The first term in the r.h.s., which seems to be of order $1/\tau$, in fact vanishes for all Φ :

$$\forall \Phi, \quad \text{Tr} \{ [\mathbb{A}, \varrho_{eq}], \Phi \} = 0. \quad (40)$$

Indeed, by using the ‘‘cyclicity of trace’’ property

$$\text{Tr} \{ [a, b] c \} = \text{Tr} \{ [c, a] b \} = \text{Tr} \{ [b, c] a \}, \quad (41)$$

and the commutativity of the diagonal multiplication operators Φ and \mathbb{A} , we have

$$\text{Tr} \{ [\mathbb{A}, \varrho_{eq}] \Phi \} = \text{Tr} \{ [\Phi, \mathbb{A}] \varrho_{eq} \} = 0.$$

Let us now simplify the second term in the r.h.s. of (39). Using the Jacobi identity

$$[a, [b, c]] + [c, [a, b]] + [b, [c, a]] = 0, \quad (42)$$

we get

$$\begin{aligned} \text{Tr} \{ [H_\varepsilon, [\mathbb{A}, \varrho_{eq}]] \Phi \} &= -\text{Tr} \{ [\varrho_{eq}, [H_\varepsilon, \mathbb{A}]] \Phi \} - \text{Tr} \{ [\mathbb{A}, [\varrho_{eq}, H_\varepsilon]] \Phi \} \\ &= -\text{Tr} \{ [[H_\varepsilon, \mathbb{A}], \Phi] \varrho_{eq} \} - \text{Tr} \{ [\Phi, \mathbb{A}] [\varrho_{eq}, H_\varepsilon] \}. \end{aligned}$$

Therefore, using again $[\Phi, \mathbb{A}] = 0$, we see that Eq. (39) reduces to

$$\text{Tr} \{ \partial_t \varrho^\tau \Phi \} = -\frac{1}{\varepsilon^2} \text{Tr} \{ [[H_\varepsilon, \mathbb{A}], \Phi] \varrho_{eq} \} + \mathcal{O}(\tau), \quad (43)$$

which must hold for every couple of test functions φ , and φ_2 . Neglecting the $\mathcal{O}(\tau)$ term, Eq. (43) is already the zeroth-order quantum ‘‘diffusive’’ model we are looking for. However, in order to show that this can be written in

the more explicit form (22), a little effort is still necessary. Using (29) and (30), we can write

$$\begin{aligned} \frac{1}{\varepsilon^2} [H_\varepsilon, \mathbb{A}] &= -\frac{1}{2} [\Delta I, \mathbb{A}] + \frac{1}{\varepsilon^2} [\phi I, \mathbb{A}] + \alpha [\mathbb{B}, \mathbb{A}] = -\frac{1}{2} [\Delta I, \mathbb{A}] + \alpha [\mathbb{B}, \mathbb{A}] \\ &= -\frac{1}{2} \begin{pmatrix} \Delta A_1 + 2\nabla A_1 \cdot \nabla & 0 \\ 0 & \Delta A_2 + 2\nabla A_2 \cdot \nabla \end{pmatrix} \\ &\quad + \alpha \begin{pmatrix} 0 & \mathcal{D}A_2 + (A_2 - A_1)\mathcal{D} \\ \mathcal{D}^*A_1 + (A_1 - A_2)\mathcal{D}^* & 0 \end{pmatrix} \end{aligned}$$

and then

$$\begin{aligned} \frac{1}{\varepsilon^2} [[H_\varepsilon, \mathbb{A}], \Phi] &= - \begin{pmatrix} \nabla A_1 \cdot \nabla \varphi_1 & 0 \\ 0 & \nabla A_2 \cdot \nabla \varphi_2 \end{pmatrix} \\ &\quad + \alpha \begin{pmatrix} 0 & (\varphi_2 - \varphi_1)\mathcal{D}A_2 + (A_2 - A_1)\mathcal{D}\varphi_2 \\ (\varphi_1 - \varphi_2)\mathcal{D}^*A_1 + (A_1 - A_2)\mathcal{D}^*\varphi_1 & 0 \end{pmatrix} \\ &\quad + \alpha \begin{pmatrix} 0 & (\varphi_1 - \varphi_2)(A_1 - A_2)\mathcal{D} \\ (\varphi_1 - \varphi_2)(A_1 - A_2)\mathcal{D}^* & 0 \end{pmatrix}. \quad (44) \end{aligned}$$

Now, from (12) and (21) we get

$$\begin{aligned} \text{Tr} \left\{ \begin{pmatrix} \nabla A_1 \cdot \nabla \varphi_1 & 0 \\ 0 & \nabla A_2 \cdot \nabla \varphi_2 \end{pmatrix} \varrho_{eq} \right\} &= \int_{\mathbb{R}^2} n_1 \nabla A_1 \cdot \nabla \varphi_1 + n_2 \nabla A_2 \cdot \nabla \varphi_2 \, d\mathbf{x} \\ &= - \int_{\mathbb{R}^2} \varphi_1 \, \text{div}(n_1 \nabla A_1) + \varphi_2 \, \text{div}(n_2 \nabla A_2) \, d\mathbf{x} \quad (45) \end{aligned}$$

and

$$\begin{aligned} &\text{Tr} \left\{ \begin{pmatrix} 0 & (\varphi_2 - \varphi_1)\mathcal{D}A_2 + (A_2 - A_1)\mathcal{D}\varphi_2 \\ (\varphi_1 - \varphi_2)\mathcal{D}^*A_1 + (A_1 - A_2)\mathcal{D}^*\varphi_1 & 0 \end{pmatrix} \varrho_{eq} \right\} \\ &= \int [(\varphi_2 - \varphi_1)\mathcal{D}A_2 + (A_2 - A_1)\mathcal{D}\varphi_2] n_{21} + [(\varphi_1 - \varphi_2)\mathcal{D}^*A_1 + (A_1 - A_2)\mathcal{D}^*\varphi_1] n_{12} \, d\mathbf{x} \\ &= \int (\varphi_2 - \varphi_1)(\mathcal{D}A_2 n_{21} - \mathcal{D}^*A_1 n_{12}) - \varphi_2 \mathcal{D}[(A_2 - A_1)n_{21}] - \varphi_1 \mathcal{D}^*[(A_1 - A_2)n_{12}] \, d\mathbf{x} \\ &= \int \varphi_2 [2 \text{Re}(\mathcal{D}A_1 n_{21}) + (A_2 - A_1)\mathcal{D}n_{21}] - \varphi_1 [2 \text{Re}(\mathcal{D}A_2 n_{21}) + (A_1 - A_2)\overline{\mathcal{D}n_{21}}] \, d\mathbf{x}, \quad (46) \end{aligned}$$

where we used $n_{21} = \overline{n_{12}}$ and $\mathcal{D}^*n_{12} = -\overline{\mathcal{D}n_{21}}$, and the integrals are extended to $\mathbf{x} \in \mathbb{R}^2$.

In order to correctly interpret also the third term in the right-hand side of Eq. (44) we note that, from definition (10), if ϱ is a scalar density operator

and ψ a scalar function, we can write

$$\begin{aligned} \operatorname{Tr} \{ \psi \mathcal{D} \varrho \} &= \operatorname{Tr} \{ (\psi, -i\psi) \cdot \nabla \varrho \} = \\ &= \operatorname{Tr} \left\{ \left[(\psi, -i\psi) \cdot \nabla + \frac{1}{2} \operatorname{div}(\psi, -i\psi) - \frac{1}{2} \operatorname{div}(\psi, -i\psi) \right] \varrho \right\} \\ &= \frac{i}{\varepsilon} \int_{\mathbb{R}^2} \psi (J_x - iJ_y) d\mathbf{x} - \frac{1}{2} \int_{\mathbb{R}^2} \mathcal{D}\psi n d\mathbf{x} \end{aligned}$$

and, similarly,

$$\operatorname{Tr} \{ \psi \mathcal{D}^* \varrho \} = -\frac{i}{\varepsilon} \int_{\mathbb{R}^2} \psi (J_x + iJ_y) d\mathbf{x} - \frac{1}{2} \int_{\mathbb{R}^2} \mathcal{D}^* \psi n d\mathbf{x}.$$

Thus:

$$\begin{aligned} &\operatorname{Tr} \left\{ \begin{pmatrix} 0 & (\varphi_1 - \varphi_2)(A_1 - A_2)\mathcal{D} \\ (\varphi_1 - \varphi_2)(A_1 - A_2)\mathcal{D}^* & 0 \end{pmatrix} \varrho_{eq} \right\} \\ &= \frac{i}{\varepsilon} \int (\varphi_1 - \varphi_2)(A_1 - A_2)(J_x^{21} - iJ_y^{21}) - (\varphi_1 - \varphi_2)(A_1 - A_2)(J_x^{12} + iJ_y^{12}) d\mathbf{x} \\ &\quad - \frac{1}{2} \int \mathcal{D} [(\varphi_1 - \varphi_2)(A_1 - A_2)] n_{21} + \mathcal{D}^* [(\varphi_1 - \varphi_2)(A_1 - A_2)] n_{12} d\mathbf{x} \\ &= \int (\varphi_1 - \varphi_2)(A_1 - A_2) \left[-\frac{2}{\varepsilon} \operatorname{Im}(J_x^{21} - iJ_y^{21}) + i \operatorname{Im} \mathcal{D} n_{21} \right] d\mathbf{x}. \quad (47) \end{aligned}$$

From Eqs. (44), (45), (46) and (47) we obtain

$$\begin{aligned} &\frac{1}{\varepsilon^2} \operatorname{Tr} \{ [[H_\varepsilon, \mathbb{A}], \Phi] \varrho_{eq} \} = \\ &\int_{\mathbb{R}^2} \varphi_1 \left[\operatorname{div}(n_1 \nabla A_1) - 2\alpha \operatorname{Re}(\mathcal{D} A_2 n_{21}) + (A_1 - A_2) \operatorname{Re}(\mathcal{D} n_{21}) - \frac{2\alpha}{\varepsilon} (A_1 - A_2) \operatorname{Im}(J_x^{21} - iJ_y^{21}) \right] d\mathbf{x} \\ &+ \int_{\mathbb{R}^2} \varphi_2 \left[\operatorname{div}(n_2 \nabla A_2) + 2\alpha \operatorname{Re}(\mathcal{D} A_1 n_{21}) + (A_1 - A_2) \operatorname{Re}(\mathcal{D} n_{21}) + \frac{2\alpha}{\varepsilon} (A_1 - A_2) \operatorname{Im}(J_x^{21} - iJ_y^{21}) \right] d\mathbf{x} \end{aligned}$$

and then, from Eq. (43) (neglecting the term $\mathcal{O}(\tau)$), we finally obtain Eq. (22).

Passing to Eq. (24) is straightforward.

3.2. Semiclassical expansion of the local equilibrium. In the following Section 3.3 we shall expand the quantum diffusive model (22) semiclassically, i.e., in powers of ε , up to order ε^2 . We remark that the parameter ε appears explicitly in equation (22) but it is also contained in all the quantities, such as A_1 , A_2 and $J_x^{21} - iJ_y^{21}$, that are computed on the local equilibrium state $\varrho_{eq} = M_{n_1 n_2} = \exp \left\{ -\frac{H_\varepsilon^A}{\varepsilon} \right\}$. Thus, we need to compute some terms of the semiclassical expansion of the local equilibrium

$$\varrho_{eq} = \varrho_{eq}^{(0)} + \varepsilon \varrho_{eq}^{(1)} + \varepsilon^2 \varrho_{eq}^{(2)} + \dots$$

As already remarked in Section 2.3, because of the factor $1/\varepsilon$ multiplying some terms in Eq. (22), if we are expanding the model up to order 2 then

we need to know (at least something about) the third-order term $\varrho_{eq}^{(3)}$. To this aim, it will be convenient to switch to the Wigner representation.

First of all we remark that $\varrho_{eq} = \varrho_{eq}(\beta = 1)$, where

$$\varrho_{eq}(\beta) = \exp(-\beta H_\varepsilon^A)$$

satisfies the semigroup equation

$$\partial_\beta \varrho_{eq}(\beta) = -H_\varepsilon^A \varrho_{eq}(\beta), \quad \varrho_{eq}(0) = I.$$

Let now $w(\beta)$ be the (matrix) Wigner function associated to $\varrho_{eq}(\beta)$ (see definition (8)). Then $w(\beta)$ satisfies

$$\partial_\beta w(\beta) = -H_\varepsilon \#_\varepsilon w(\beta), \quad w(0) = I, \quad (48)$$

where $\#$ is the Weyl-Moyal product (also known as “twisted product”) [17] and H_ε denotes here the symbol of the Hamiltonian H_ε^A , i.e.

$$\begin{aligned} H_\varepsilon(\mathbf{x}, \mathbf{p}) &= \begin{pmatrix} \frac{1}{2}p^2 + \mu_1(\mathbf{x}) & 0 \\ 0 & \frac{1}{2}p^2 + \mu_2(\mathbf{x}) \end{pmatrix} + \varepsilon \alpha \begin{pmatrix} 0 & p_y + ip_x \\ p_y - ip_x & 0 \end{pmatrix} \\ &=: H_0(\mathbf{x}, \mathbf{p}) + \varepsilon H_1(\mathbf{x}, \mathbf{p}), \end{aligned} \quad (49)$$

where

$$\mu_j(\mathbf{x}) = \phi(\mathbf{x}) + A_j(\mathbf{x}), \quad j = 1, 2, \quad (50)$$

and, of course, $p^2 = |\mathbf{p}|^2 = p_x^2 + p_y^2$. Moreover, the Weyl-Moyal product has a well known formal expansion in powers of ε :

$$A \#_\varepsilon B = \sum_{k=0}^{\infty} \frac{\varepsilon^k}{(2i)^k} \sum_{|r|+|s|=k} \frac{(-1)^{|r|}}{r! s!} (\partial_{\mathbf{x}}^r \partial_{\mathbf{p}}^s A) (\partial_{\mathbf{p}}^r \partial_{\mathbf{x}}^s B) =: \sum_{k=0}^{\infty} \varepsilon^k A \#_k B, \quad (51)$$

where we introduced the compact notation $\partial_{\boldsymbol{\xi}}^j = \partial/\partial \xi_j$. Expanding also $w(\beta)$ in powers of ε ,

$$w(\beta) = w^{(0)}(\beta) + \varepsilon w^{(1)}(\beta) + \varepsilon^2 w^{(2)}(\beta) + \dots,$$

and comparing right and hand sides of Eq. (48), we obtain

$$\begin{cases} \partial_\beta w^{(k)}(\beta) = -H_0 w^{(k)}(\beta) - \sum_{j=1}^k \left[H_0 \#_j w^{(k-j)}(\beta) + H_1 \#_{j-1} w^{(k-j)}(\beta) \right], \\ w^{(0)}(0) = I, \quad w^{(k)}(0) = 0, \quad k \geq 1, \end{cases} \quad (52)$$

(where we used $H_0 \#_0 w^{(k)} = H_0 w^{(k)}$). Finally, let

$$\hat{w}(z) = \mathcal{L}[w](z)$$

denote the Laplace transform of $w(\beta)$. Then, from (52) we obtain

$$\begin{cases} \hat{w}^{(0)}(z) = R(z), \\ \hat{w}^{(k)}(z) = - \sum_{j=1}^k R(z) \left[H_0 \#_j \hat{w}^{(k-j)}(z) + H_1 \#_{j-1} \hat{w}^{(k-j)}(z) \right], \quad k \geq 1, \end{cases} \quad (53)$$

where

$$R(z) = (z + H_0)^{-1} = \begin{pmatrix} (z + \frac{1}{2}p^2 + \mu_1)^{-1} & 0 \\ 0 & (z + \frac{1}{2}p^2 + \mu_2)^{-1} \end{pmatrix} =: \begin{pmatrix} R_1(z) & 0 \\ 0 & R_2(z) \end{pmatrix}. \quad (54)$$

Recalling the Laplace inversion formula

$$\mathcal{L}^{-1} [(z + f)^{-n}] (\beta) = \frac{e^{-\beta f} \beta^{n-1}}{(n-1)!}, \quad (55)$$

the zeroth order approximation to the local equilibrium is

$$w^{(0)}(\beta) = \mathcal{L}^{-1} [R] (\beta) = \begin{pmatrix} e^{-\beta(\frac{1}{2}p^2 + \mu_1)} & 0 \\ 0 & e^{-\beta(\frac{1}{2}p^2 + \mu_2)} \end{pmatrix}, \quad (56)$$

that is (as it was expected) two independent classical Maxwellians, one for each spin population.

At first order we have

$$\begin{aligned} \hat{w}^{(1)}(z) &= -R(z) [H_0 \#_1 \hat{w}^{(0)}(z) + H_1 \hat{w}^{(0)}(z)] \\ &= -R(z) [H_0 \#_1 R(z) + H_1 R(z)] = -R(z) H_1 R(z), \end{aligned}$$

where $H_0 \#_1 R(z) = 0$ follows from $R(z) = (z + H_0)^{-1}$ (and, therefore, $R(z)$ is a function of H_0) and from the fact that $\#_1$ is a Poisson bracket:

$$A \#_1 B = \frac{i}{2} (\nabla_{\mathbf{x}} A \cdot \nabla_{\mathbf{p}} B - \nabla_{\mathbf{p}} A \cdot \nabla_{\mathbf{x}} B)$$

(see (51)). Hence,

$$\hat{w}^{(1)}(z) = -\alpha \begin{pmatrix} 0 & (p_y + ip_x) \\ (p_y - ip_x) & 0 \end{pmatrix} R_1(z) R_2(z). \quad (57)$$

The inverse Laplace transform of $R_1(z) R_2(z)$ can be computed by factorization. More in general, the inverse Laplace transform of

$$R_1^r(z) R_2^s(z) = \frac{1}{(z + f_1)^r (z + f_2)^s},$$

with $f_i = \frac{1}{2}p^2 + \mu_i$, can be computed by using the factorization formula

$$\frac{1}{(z + f_1)^r (z + f_2)^s} = \sum_{k=0}^{r-1} \frac{a_k(r, s)}{(f_2 - f_1)^{s+k} (z + f_1)^{r-k}} + \sum_{k=0}^{s-1} \frac{b_k(r, s)}{(f_1 - f_2)^{r+k} (z + f_2)^{s-k}}$$

where the coefficients $a_k = a_k(r, s)$, $b_k = b_k(r, s)$ are recursively given by

$$\begin{cases} a_0 = 1 \\ a_k = - \sum_{j=\max\{0, k-s\}}^{k-1} \binom{s}{k-j} a_j, & k = 1, \dots, r-1, \\ b_0 = 1 \\ b_k = - \sum_{j=\max\{0, k-r\}}^{k-1} \binom{r}{k-j} b_j, & k = 1, \dots, s-1. \end{cases} \quad (58)$$

Using the inversion formula (55) with $\beta = 1$ we find, therefore,

$$\mathcal{L}^{-1} [R_1^r R_2^s] (\beta = 1) = R_{rs}(\mu_1, \mu_2) e^{-p^2/2}, \quad (59)$$

where

$$R_{rs}(\mu_1, \mu_2) = \sum_{k=0}^{r-1} \frac{a_k(r, s) e^{-\mu_1}}{(r-k-1)! (\mu_2 - \mu_1)^{s+k}} + \sum_{k=0}^{s-1} \frac{b_k(r, s) e^{-\mu_2}}{(s-k-1)! (\mu_1 - \mu_2)^{r+k}}. \quad (60)$$

It will be useful to write this expression in some particular cases:

$$\begin{aligned} R_{r0}(\mu_1, \mu_2) &= \frac{e^{-\mu_1}}{(r-1)!}, \\ R_{r1}(\mu_1, \mu_2) &= \frac{e^{-\mu_2} - e^{-\mu_1}}{(\mu_1 - \mu_2)^r} - \sum_{k=0}^{r-2} \frac{e^{-\mu_1}}{(r-k-1)! (\mu_1 - \mu_2)^{k+1}} \quad (61) \\ R_{rr}(\mu_1, \mu_2) &= \sum_{k=0}^{r-1} \frac{a_k(r, r) (e^{-\mu_1} + (-1)^{r+k} e^{-\mu_2})}{(r-k-1)! (\mu_2 - \mu_1)^{r+k}}. \end{aligned}$$

Other expressions, such as those of R_{0s} and R_{1s} , can be obtained by means of the relation

$$R_{rs}(\mu_1, \mu_2) = R_{sr}(\mu_2, \mu_1). \quad (62)$$

Coming back to (57), we easily obtain

$$\mathcal{L}^{-1}[R_1 R_2](\beta = 1) = R_{11}(\mu_1, \mu_2) e^{-p^2/2} = \frac{e^{-\mu_1} - e^{-\mu_2}}{\mu_2 - \mu_1} e^{-p^2/2}$$

and then

$$w^{(1)}(\beta = 1) = \alpha \begin{pmatrix} 0 & (p_y + ip_x) \\ (p_y - ip_x) & 0 \end{pmatrix} \frac{e^{-\mu_1} - e^{-\mu_2}}{\mu_1 - \mu_2} e^{-p^2/2}. \quad (63)$$

In the same way one can compute higher order terms, which are more and more complicated. However, thanks to the property

$$\nabla_{\mathbf{x}} R_j = -R_j^2 \nabla_{\mathbf{x}} \mu_j, \quad \nabla_{\mathbf{p}} R_j = -R_j^2 \mathbf{p}, \quad j = 1, 2,$$

each term will be a linear combinations of the above defined functions R_{rs} . For example, for the second order term

$$\hat{w}^{(2)} = R[H_0 \#_1 (RH_1 R) + H_1 R H_1 R - H_0 \#_2 R - H_1 \#_1 R],$$

we get

$$\begin{aligned} w_{11}^{(2)}(\beta = 1) &= \frac{e^{-p^2/2}}{4} \left[R_{40} (|\nabla \mu_1|^2 + (\mathbf{p} \cdot \nabla)^2 \mu_1) - R_{30} \Delta \mu_1 + 4\alpha^2 p^2 R_{21} \right], \\ w_{22}^{(2)}(\beta = 1) &= \frac{e^{-p^2/2}}{4} \left[R_{04} (|\nabla \mu_2|^2 + (\mathbf{p} \cdot \nabla)^2 \mu_2) - R_{03} \Delta \mu_2 + 4\alpha^2 p^2 R_{12} \right], \\ w_{21}^{(2)}(\beta = 1) &= \frac{i\alpha e^{-p^2/2}}{2} \left[R_{21} (i\partial_x - \partial_y) \mu_1 - R_{12} (i\partial_x - \partial_y) \mu_2 - R_{22} (ip_x - p_y) \mathbf{p} \cdot \nabla (\mu_1 - \mu_2) \right], \\ w_{12}^{(2)} &= \bar{w}_{21}^{(2)}, \end{aligned} \quad (64)$$

where the explicit expressions of the various R_{rs} can be easily obtained from Eqs. (60) and (62).

Much more effort is required to compute the third order term from

$$\hat{w}^{(3)} = R[H_0 \#_1 \hat{w}^{(2)} + H_0 \#_2 \hat{w}^{(1)} + H_0 \#_3 \hat{w}^{(0)} + H_1 \#_0 \hat{w}^{(2)} + H_1 \#_1 \hat{w}^{(1)} + H_1 \#_2 \hat{w}^{(0)}].$$

Looking at (22) we see that, if we want to expand the diffusive model up to second order in ε , then $w^{(3)}$ enters through the third-order current term

$$\text{Im}(J_x^{21} - iJ_y^{21})^{(3)} = \text{Im} \int_{\mathbb{R}^2} (p_x - ip_y) w_{21}^{(3)}(\mathbf{x}, \mathbf{p}) d\mathbf{p}.$$

It turns out that the only non-zero contribution comes from $R[H_0\#_1\hat{w}^{(2)} + H_0\#_2\hat{w}^{(1)} + H_1\#_0\hat{w}^{(2)}]$ and is given by

$$\begin{aligned} \text{Im} \int_{\mathbb{R}^2} (p_x - ip_y) w_{21}^{(3)}(\mathbf{x}, \mathbf{p}) d\mathbf{p} = \\ \frac{c\alpha}{2} \left\{ (2R_{41} - R_{31} - R_{22} + 2R_{23}) \Delta\mu_1 + (2R_{32} + R_{41} - 4R_{33}) |\nabla\mu_1|^2 \right. \\ \left. + (2R_{14} - R_{13} - R_{22} + 2R_{32}) \Delta\mu_2 + (2R_{23} + R_{14} - 4R_{33}) |\nabla\mu_2|^2 \right. \\ \left. + (8R_{33} - R_{32} - R_{23}) \nabla\mu_1 \cdot \nabla\mu_2 + 16\alpha^2 R_{22} \right\}, \end{aligned} \quad (65)$$

where we have put

$$c = \int_{\mathbb{R}^2} e^{-p^2/2} d\mathbf{p} = 2\pi. \quad (66)$$

3.3. Semiclassical expansion of the diffusive model. We can now apply the results of the preceding section to expand the diffusive model (22) in powers of ε up to ε^2 . This will eventually yield Eq. (27) and, therefore, Theorem 2.

To this end, what we have to do is expanding

$$\begin{aligned} A_j(n_1, n_2) &= A_j^{(0)}(n_1, n_2) + \varepsilon A_j^{(1)}(n_1, n_2) + \varepsilon^2 A_j^{(2)}(n_1, n_2) + \dots, \\ n_{21} &= n_{21}^{(0)} + \varepsilon n_{21}^{(1)} + \varepsilon^2 n_{21}^{(2)} + \dots, \\ J_x^{21} - iJ_y^{21} &= (J_x^{21} - iJ_y^{21})^{(0)} + \varepsilon (J_x^{21} - iJ_y^{21})^{(1)} + \varepsilon^2 (J_x^{21} - iJ_y^{21})^{(2)} + \dots, \end{aligned}$$

where $A_j^{(k)} = A_j^{(k)}(n_1, n_2)$, $n_{21}^{(k)} = n_{21}^{(k)}(n_1, n_2)$ and $(J_x^{21} - iJ_y^{21})^{(k)} = (J_x^{21} - iJ_y^{21})^{(k)}(n_1, n_2)$, should be computed as functions of n_1 and n_2 by using the k -th order approximation of the local equilibrium,

$$w \approx w^{(0)} + \varepsilon w^{(1)} + \dots + \varepsilon^k w^{(k)},$$

which has been investigated in the previous section. Using (56), (63) and (64) (and recalling definition (66)) we obtain

$$\int_{\mathbb{R}^2} w_{11}^{(0)} d\mathbf{p} = c e^{-\mu_1}, \quad (67a)$$

$$\int_{\mathbb{R}^2} w_{21}^{(0)} d\mathbf{p} = 0, \quad (67b)$$

$$\int_{\mathbb{R}^2} (p_x - ip_y) w_{21}^{(0)} d\mathbf{p} = 0, \quad (67c)$$

$$\int_{\mathbb{R}^2} w_{11}^{(1)} d\mathbf{p} = 0, \quad (67d)$$

$$\int_{\mathbb{R}^2} w_{21}^{(1)} d\mathbf{p} = 0, \quad (67e)$$

$$\int_{\mathbb{R}^2} \text{Im}(p_x - ip_y) w_{21}^{(1)} d\mathbf{p} = 2c\alpha R_{11} = 2c\alpha \frac{e^{-\mu_1} - e^{-\mu_2}}{\mu_2 - \mu_1}, \quad (67f)$$

$$\int_{\mathbb{R}^2} w_{11}^{(2)} d\mathbf{p} = c e^{-\mu_1} \left(\frac{1}{24} |\nabla \mu_1|^2 - \frac{1}{12} \Delta \mu_1 \right) + 2c\alpha^2 R_{21}, \quad (67g)$$

$$\int_{\mathbb{R}^2} w_{21}^{(2)} d\mathbf{p} = \frac{ic\alpha}{2} [(R_{21} - R_{22})(i\partial_x - \partial_y)\mu_1 - (R_{12} - R_{22})(i\partial_x - \partial_y)\mu_2], \quad (67h)$$

$$\int_{\mathbb{R}^2} (p_x - ip_y) w_{21}^{(2)} d\mathbf{p} = 0, \quad (67i)$$

while $\text{Im} \int_{\mathbb{R}^3} (p_x - ip_y) w_{21}^{(2)} d\mathbf{p}$ is given by (65). The moments of $w_{22}^{(k)}$ can be obtained by the corresponding moments of $w_{22}^{(k)}$ (Eqs. (67a), (67d) and (67g)) by changing 1 into 2 and 2 into 1.

From (67a) we see that the relation between chemical potentials and spin densities at order 0 is

$$n_j = c e^{-\mu_j} = c e^{-\phi - A_j}, \quad j = 1, 2,$$

and then

$$\mu_j^{(0)}(n_1, n_2) = -\log \frac{n_j}{c}, \quad A_j^{(0)} = \mu_j^{(0)} - \phi, \quad j = 1, 2. \quad (68)$$

At first order, we see from Eq. (67d) that the relation between densities and chemical potentials remains unchanged, and is still given by (68). Moreover, from (67b) we see that the terms containing n_{21} vanish in (22) at order 0 while, because of the factor ε^{-1} , the current contribution comes from $\text{Im}(J_x^{21} - iJ_y^{21})^{(1)}$. Using (67f) and (68) we get

$$\text{Im}(J_x^{21} - iJ_y^{21})^{(1)} = 2c\alpha \frac{e^{-\mu_1} - e^{-\mu_2}}{\mu_2 - \mu_1} = 2\alpha \frac{n_1 - n_2}{A_2 - A_1}. \quad (69)$$

The resulting zeroth order approximation in ε of the quantum diffusive model (22) is

$$\begin{aligned}\partial_t n_1 - \operatorname{div}(\nabla n_1 + n_1 \nabla \phi) &= 4\alpha^2(n_2 - n_1) \\ \partial_t n_2 - \operatorname{div}(\nabla n_2 + n_2 \nabla \phi) &= 4\alpha^2(n_1 - n_2)\end{aligned}\tag{70}$$

As already noticed in Sec. 2.3, this is a drift-diffusion system with a coupling term of D'yakonov-Perel' type [30].

Moreover, from Eqs. (67e) and (67i) we see that the contributions from n_{21} and $\operatorname{Im}(J_x^{21} - iJ_y^{21})^{(2)}$ vanish. Hence, the drift-diffusion system (70) is still correct at first order in ε .

If we want to invert at second order in ε the relation between μ_j and n_j , we can use (67a), (67d) and (67g) to write

$$n_1 = c e^{-\mu_1} \left[1 + \varepsilon^2 \left(\frac{|\nabla \mu_1|^2}{24} - \frac{\Delta \mu_1}{12} + 2\alpha^2 e^{\mu_1} R_{21}(\mu_1, \mu_2) \right) \right] + o(\varepsilon^2)$$

and then

$$n_1 = c e^{-\mu_1} \left[1 + \varepsilon^2 \left(\frac{|\nabla \mu_1^{(0)}|^2}{24} - \frac{\Delta \mu_1^{(0)}}{12} + 2\alpha^2 e^{\mu_1^{(0)}} R_{21}^{(0)}(\mu_1, \mu_2) \right) \right] + o(\varepsilon^2).$$

Using (68), therefore, we obtain

$$n_1 = c e^{-\mu_1} \left[1 + \varepsilon^2 \left(\frac{|\nabla \log n_1|^2}{24} + \frac{\Delta \log n_1}{12} + \frac{2\alpha^2}{n_1} S_{21}(n_1, n_2) \right) \right] + o(\varepsilon^2),$$

where we put

$$S_{rs}(n_1, n_2) := c R_{rs}^{(0)}(\mu_1, \mu_2) = c R_{rs}(\mu_1^{(0)}, \mu_2^{(0)}) = R_{rs}(-\log n_1, -\log n_2)\tag{71}$$

(recall that R_{rs} has been defined in (60)). Hence, we obtain that at order ε^2 the following relation between μ_1 and n_1 holds:

$$e^{\mu_1} = \frac{c}{n_1} \left[1 + \varepsilon^2 \left(\frac{|\nabla \log n_1|^2}{24} + \frac{\Delta \log n_1}{12} + \frac{2\alpha^2}{n_1} S_{21}(n_1, n_2) \right) \right],\tag{72}$$

which implies

$$\mu_1^{(2)}(n_1, n_2) = A^{(2)}(n_1, n_2) = Q(n_1) + \frac{2\alpha^2}{n_1} S_{21}(n_1, n_2),\tag{73}$$

(the same for μ_2 and n_2 after changing 1,2 into 2,1), where we introduced the Bohm potential

$$Q(n_i) = \frac{|\nabla \log n_i|^2}{24} + \frac{\Delta \log n_i}{12} = \frac{1}{6} \frac{\Delta \sqrt{n_i}}{\sqrt{n_i}}.\tag{74}$$

From (67b), (67c), (67e) and (67i), we see that the only non-vanishing ε^2 -order terms in Eqs. (22) are:

$$\begin{aligned}\operatorname{div}(n_1 \nabla A_1^{(2)}) + \alpha(A_1 - A_2)^{(0)} \operatorname{Re}(\mathcal{D}n_{21}^{(2)}) - 2\alpha \operatorname{Re}(n_{21}^{(2)} \mathcal{D}A_2^{(0)}) \\ - 2\alpha(A_1 - A_2)^{(2)} \operatorname{Im}(J_x^{21} - iJ_y^{21})^{(1)} - 2\alpha(A_1 - A_2)^{(0)} \operatorname{Im}(J_x^{21} - iJ_y^{21})^{(3)}.\end{aligned}$$

By using the expressions of $A_j^{(0)}$, $A_j^{(2)}$, $n_{21}^{(2)}$, $\text{Im}(J_x^{21} - iJ_y^{21})^{(1)}$ and $\text{Im}(J_x^{21} - iJ_y^{21})^{(3)}$ given, respectively, by (68), (73), (67h), (69) and (65), and recalling that $S_{rs} = S_{rs}(n_1, n_2)$ is given by (71), we obtain

$$\text{div}(n_1 \nabla A_1^{(2)}) = \text{div} \left\{ n_1 \nabla \left[Q(n_1) + \frac{2\alpha^2}{n_1} S_{21} \right] \right\},$$

$$\begin{aligned} & \alpha(A_1 - A_2)^{(0)} \text{Re}(\mathcal{D}n_{21}^{(2)}) = \\ & \frac{c\alpha^2}{2} \log \frac{n_1}{n_2} \text{Re} \left\{ (\partial_x - i\partial_y)(R_{21} - R_{22})^{(0)} (\partial_x + i\partial_y)\mu_1^{(0)} - (\partial_x - i\partial_y)(R_{12} - R_{22})^{(0)} (\partial_x + i\partial_y)\mu_2^{(0)} \right\} \\ & = \frac{\alpha^2}{2} \log \frac{n_1}{n_2} \text{Re} \left\{ (\partial_x - i\partial_y)(S_{22} - S_{21})(\partial_x + i\partial_y) \log n_1 - (\partial_x - i\partial_y)(S_{22} - S_{21})(\partial_x + i\partial_y) \log n_2 \right\} \\ & = \frac{\alpha^2}{2} \log \frac{n_1}{n_2} \text{div} \left\{ S_{12} \nabla \log n_2 - S_{21} \nabla \log n_1 + S_{22} \nabla \log \frac{n_1}{n_2} \right\}, \end{aligned}$$

$$\begin{aligned} & 2\alpha \text{Re}(n_{21}^{(2)} \mathcal{D}A_2^{(0)}) = \\ & c\alpha^2 [(R_{21} - R_{22})^{(0)} (\partial_x + i\partial_y)\mu_1^{(0)} - (R_{12} - R_{22})^{(0)} \mu_2^{(0)}] (\partial_x + i\partial_y) (\log n_2 + \phi) \\ & = \alpha^2 \left\{ S_{12} \nabla \log n_2 - S_{21} \nabla \log n_1 + S_{22} \nabla \log \frac{n_1}{n_2} \right\} \cdot \nabla (\phi + \log n_2), \end{aligned}$$

$$\begin{aligned} & 2\alpha(A_1 - A_2)^{(2)} \text{Im}(J_x^{21} - iJ_y^{21})^{(1)} = \\ & 4c\alpha^2 \left[Q(n_1) - Q(n_2) + \frac{2\alpha^2}{n_1} S_{21} - \frac{2\alpha^2}{n_2} S_{12} \right] R_{11}^{(0)} \\ & = 4\alpha^2 [Q(n_1) - Q(n_2)] S_{11} + 8\alpha^4 \left(\frac{S_{21}}{n_1} - \frac{S_{12}}{n_2} \right) S_{11} \end{aligned}$$

$$\begin{aligned} & 2\alpha(A_1 - A_2)^{(0)} \text{Im}(J_x^{21} - iJ_y^{21})^{(3)} = \\ & -\alpha^2 \log \frac{n_1}{n_2} \left\{ (S_{22} + S_{31} - 2S_{23} - 2S_{41}) \Delta \log n_1 + (S_{22} + S_{13} - 2S_{32} - 2S_{14}) \Delta \log n_2 \right. \\ & \quad + (2S_{32} + S_{41} - 4S_{33}) |\nabla \log n_1|^2 + (2S_{23} + S_{14} - 4S_{33}) |\nabla \log n_2|^2 \\ & \quad \left. + (8S_{33} - S_{32} - S_{23}) \nabla \log n_1 \cdot \nabla \log n_2 + 16\alpha^2 S_{22} \right\}. \end{aligned}$$

We see, therefore, that the second-order semiclassical approximation of the quantum drift-diffusion equations (22) is given by (27) with

$$\begin{aligned}
C_1(n_1, n_2) &= 2 \operatorname{div} \left(n_1 \nabla \frac{S_{21}}{n_1} \right) - 4 [Q(n_1) - Q(n_2)] S_{11} \\
&+ \frac{1}{2} \log \frac{n_1}{n_2} \operatorname{div} \left(S_{12} \nabla \log n_2 - S_{21} \nabla \log n_1 + S_{22} \nabla \log \frac{n_1}{n_2} \right) \\
&- \nabla(\phi + \log n_2) \cdot \left(S_{12} \nabla \log n_2 - S_{21} \nabla \log n_1 + S_{22} \nabla \log \frac{n_1}{n_2} \right) \\
&+ \log \frac{n_1}{n_2} \left\{ (S_{22} + S_{31} - 2S_{23} - 2S_{41}) \Delta \log n_1 + (S_{22} + S_{13} - 2S_{32} - 2S_{14}) \Delta \log n_2 \right. \\
&\quad \left. + (2S_{32} + S_{41} - 4S_{33}) |\nabla \log n_1|^2 + (2S_{23} + S_{14} - 4S_{33}) |\nabla \log n_2|^2 \right. \\
&\quad \left. + (8S_{33} - S_{32} - S_{23}) \nabla \log n_1 \cdot \nabla \log n_2 \right\}
\end{aligned} \tag{75}$$

and

$$C_2(n_1, n_2) = 16S_{22} \log \frac{n_1}{n_2} - 8S_{11} \left(\frac{S_{21}}{n_1} - \frac{S_{12}}{n_2} \right). \tag{76}$$

This proves Theorem 2. For the sake of completeness, let us give the explicit expressions for the S_{rs} terms that interfere in (75) and (76). They are obtained by the corresponding R_{rs} terms through the definition $S_{rs}(n_1, n_2) = R_{rs}(-\log n_1, -\log n_2)$. By using (58), (60) and (61), it is not difficult to obtain the following expressions:

$$R_{11}(\mu_1, \mu_2) = \frac{e^{-\mu_1} - e^{-\mu_2}}{\mu_2 - \mu_1},$$

$$R_{21}(\mu_1, \mu_2) = \frac{e^{-\mu_1}}{\mu_2 - \mu_1} - \frac{e^{-\mu_1} - e^{-\mu_2}}{(\mu_2 - \mu_1)^2},$$

$$R_{22}(\mu_1, \mu_2) = \frac{e^{-\mu_1} + e^{-\mu_2}}{(\mu_2 - \mu_1)^2} - \frac{2(e^{-\mu_1} - e^{-\mu_2})}{(\mu_2 - \mu_1)^3},$$

$$R_{31}(\mu_1, \mu_2) = \frac{e^{-\mu_1}}{2(\mu_2 - \mu_1)} - \frac{e^{-\mu_1}}{(\mu_2 - \mu_1)^2} + \frac{e^{-\mu_1} - e^{-\mu_2}}{(\mu_2 - \mu_1)^3},$$

$$R_{32}(\mu_1, \mu_2) = \frac{e^{-\mu_1}}{2(\mu_2 - \mu_1)^2} - \frac{2e^{-\mu_1} + e^{-\mu_2}}{(\mu_2 - \mu_1)^3} + \frac{3(e^{-\mu_1} - e^{-\mu_2})}{(\mu_2 - \mu_1)^4},$$

$$R_{33}(\mu_1, \mu_2) = \frac{e^{-\mu_1} - e^{-\mu_2}}{2(\mu_2 - \mu_1)^3} - \frac{3(e^{-\mu_1} + e^{-\mu_2})}{(\mu_2 - \mu_1)^4} + \frac{6(e^{-\mu_1} - e^{-\mu_2})}{(\mu_2 - \mu_1)^5},$$

$$R_{41}(\mu_1, \mu_2) = \frac{e^{-\mu_1}}{6(\mu_2 - \mu_1)} - \frac{e^{-\mu_1}}{2(\mu_2 - \mu_1)^2} + \frac{e^{-\mu_1}}{(\mu_2 - \mu_1)^3} - \frac{e^{-\mu_1} - e^{-\mu_2}}{(\mu_2 - \mu_1)^4}.$$

Reverse terms, such as R_{12} , R_{23} ecc., are simply obtained by using the relation $R_{rs}(\mu_1, \mu_2) = R_{sr}(\mu_2, \mu_1)$. **Acknowledgment.** The authors were supported by the Agence Nationale de la Recherche, ANR project QUATRAIN.

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E-mail address: `barletti@math.unifi.it`

DIPARTIMENTO DI MATEMATICA, UNIVERSITÀ DI FIRENZE, ITALIA

E-mail address: `florian.mehats@univ-rennes1.fr`

IRMAR, UNIVERSITÉ DE RENNES 1, FRANCE