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Hydrodynamic Models with Quantum Corrections

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Abstract We derive a quantum-corrected hydrodynamic and drift-diffusion model for the out-of-equilibrium particle dynamics in the presence of particle collisions, modeled by a BGK collision term. The quantum mechanical corrections are obtained within the Liouville formalism and are expressed by an effective nonlinear force. The Boltzmann and Fermi-Dirac statistics are included.

Keywords Hydrodynamical models · Quantum-corrected Liouville model

1 Introduction

By the technological progress made in the last decade on the fabrication of microelectronics devices, the active regions of integrated transistors is nowadays downscaled to the submicrometer dimensions. This opens new possibilities for designing components for high frequency and optoelectronic devices. As an example, devices based on the quantum tunneling process like the resonant tunneling diodes are currently applied in high frequency integrated oscillators. They are obtained by growing, via molecular-beam epitaxy, a succession of layers of different materials connected by abrupt junctions. As a result, the particles inside such an heterostructure material experience strong fields and discontinuous electric potentials.

Under such extremal conditions, mathematical models for particle transport in semiconductor devices cannot discard quantum effects. Various formalisms have been developed in order to describe the particle motion in a full-quantum framework. In particular, the quantum phase-space approach is a well established method for the study of the quantum evolution

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of interacting particles in a media [11, 15]. In this formalism, the Louville distribution function, that describes the motion of classical particles, is generalized to a non-positive definite distribution denoted as Wigner quasi-distribution function. The Wigner quasi-distribution shares strong similarities with the classical Liouville distribution [7, 9, 12]. In particular, the moments (weighted integrals with respect to the momentum) of the Wigner function, provide the macroscopic quantities (like particle density, current and energy), in same way of the classical formalism. Such a quasi-classical description provides some advantages in terms of simplicity in the physical interpretation and the availability of feasible method for the inclusion of irreversible processes like thermalization or phase breaking mechanisms.

However, the direct numerical discretization of the Wigner equation of motion is extremely challenging [13, 15]. The Wigner evolution equation is given in terms of some nonlocal-in-space pseudo-differential operators. Furthermore, in the same way as the classical phase-space description of the dynamics, the quantum formalism use the position and the momentum of the particles as kinetic variables. Compared with the Schrödinger approach, this choice doubles the dimension of the physical space and becomes extremely demanding from the computational and the cpu-memory point of view.

The typical strategy to reduce the complexity of such quantum-kinetic models is to derive so called quantum-fluid models which, analogously to classical fluid models, are formulated in terms of a finite number of macroscopic moments of the Wigner function (see i.e. Refs. [1, 2, 8] for the application of the method of moment to the classical systems). The equations of a quantum fluid, therefore, can be deduced from the underlying phase-space description [5, 16]. These models have been applied to different context. As an example, quantum-hydrodynamic models have been used to the reproduce the particle motion in semiconductors and some new functional materials like the graphene [4, 17]. Hydrodynamics approaches are able to capture some interesting quantum phenomena like the band transition in multiband systems [10] and the resonant tunneling in heterostructures [6].

However, the description of the full quantum dynamics at the hydrodynamical level is extremely challenging and in many cases infeasible. A common practice is to exploit the analogy between the Wigner formalism and the classical Liouville dynamics, and derive quantum corrected models that extend the validity of the conventional drift diffusion or hydrodynamic models.

The most popular approach concerns the so-called $\hbar$-expansion [5]. It is based on the observation that in the quantum phase space framework, the hamiltonian of the system is represented by a pseudo-differential operator that admits a formal h-expansion where the leading term is the usual classical hamiltonian. Although this approach appears to be the most natural way to proceed, the use of quantum corrected models based on the $\hbar$-expansion encounters many difficulties. In fact, this procedure generates a quite large number of corrective terms, and it is usually very difficult (sometime impossible) to ascribe to them a clear physical meaning.

Here, we use a different approach which is based on the quantum-corrected Liouville (QL) model described in Ref. [14]. In this context, the quantum motion is described in term of particles traveling along trajectories in the presence of an effective quantum mechanical potential. In particular, the description of the quantum motion is maintained as close as possible to the classical counterpart. The corrections to the classical trajectories are expressed by an effective nonlinear force. This effective force describes the non-local character of the quantum particles. This approach offers the considerable advantage that some quantum corrections can be easily integrated, for example, in a classical code. In Ref. [14] the particle motion was described at the kinetic level and the well posedeness of the quantum-corrected Liouville problem was investigated.

In the present contribution, the QL model is used in order to derive an hydrodynamic system that contains some quantum corrections and that can be applied to the study of the particle motion in nanometric structures.

2 Quantum Corrected Kinetic Model

We consider a spinless particle of mass m and charge q, represented by the wavefunction $|\psi\rangle$ in the presence of an electric potential V. The Wigner function f^W related to the state $|\psi\rangle$ is defined by:

$$f^W(\mathbf{x}, \mathbf{p}) = W\big[|\psi\rangle\langle\psi|\big],$$

where the Wigner operator W is

$$W\big[|\psi\rangle\langle\phi|\big] = \frac{1}{(2\pi)^3}\int \left\langle \mathbf{x} + \frac{\hbar}{2}\boldsymbol{\eta}|\psi\rangle\langle\phi|\mathbf{x} - \frac{\hbar}{2}\boldsymbol{\eta}\right\rangle e^{i\mathbf{p}\cdot\boldsymbol{\eta}}\,\mathrm{d}\boldsymbol{\eta}.$$

The evolution equation for the Wigner distribution is obtained from the Schrödinger equation

$$\frac{\partial f^W}{\partial t} + \frac{\mathbf{p}}{m}\cdot\nabla_x f^W - q\theta[V]f^W = 0, \tag{1}$$

where the pseudo-differential operator $\theta[V]$ is defined by

$$\theta[V]f = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \delta V(\mathbf{x}, \boldsymbol{\eta}) e^{i(\mathbf{p}-\bar{\mathbf{p}})\cdot\boldsymbol{\eta}} f(\mathbf{x}, \bar{\mathbf{p}})\,\mathrm{d}\boldsymbol{\eta}\,\mathrm{d}\bar{\mathbf{p}},$$

with

$$\delta V(\mathbf{x}, \boldsymbol{\eta}) = \frac{i}{\hbar}\left[V\left(\mathbf{x} + \frac{\hbar}{2}\boldsymbol{\eta}\right) - V\left(\mathbf{x} - \frac{\hbar}{2}\boldsymbol{\eta}\right)\right].$$

According to Ref. [14], our model of the particle motion has the structure of a classical Liouville equation with some quantum corrections. They are obtained by requiring that the solutions of the quantum-corrected model are the best approximation (in terms of the L^2 norm) of the solutions of the Wigner equation. We consider a model of the form:

$$\frac{\partial f}{\partial t} + \mathbf{v}^{QC}\cdot\nabla_x f + q\boldsymbol{\mathcal{E}}^{QC}\cdot\nabla_p f = 0, \tag{2}$$

and choose $\mathbf{v}^{QC}[f]$, $\boldsymbol{\mathcal{E}}^{QC}[V, f]$ in order to minimize the L^2-norm of the difference of the classical-like solution and the Wigner function,

$$\big\|f - f^W\big\|_{L^2_{x,p}}.$$

We obtain that the velocity field coincides with the classical term $\mathbf{v}^{QC} = \frac{\mathbf{p}}{m}$ and that the quantum-corrected electric field depends nonlinearly from the solution of Eq. (2) as follows

$$\mathcal{E}_j^{QC}[V, f] = \frac{\int_{\mathbb{R}^3} i\eta_j \delta V(\mathbf{x}, \boldsymbol{\eta})|\widetilde{f}(\mathbf{x}, \boldsymbol{\eta})|^2\,\mathrm{d}\boldsymbol{\eta}}{\int_{\mathbb{R}^3}\eta_j^2|\widetilde{f}(\mathbf{x}, \boldsymbol{\eta})|^2\,\mathrm{d}\boldsymbol{\eta}}, \tag{3}$$

where the tilde denotes Fourier transform with respect to $\mathbf{p}$,

$$\widetilde{f}(\mathbf{x}, \boldsymbol{\eta}) = \int_{\mathbb{R}^3} f(\mathbf{x}, \mathbf{p}) e^{-i\mathbf{p}\cdot\boldsymbol{\eta}} \, \mathrm{d}\mathbf{p}.$$

The hydrodynamic equations are obtained from the following quantum-corrected kinetic model

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla_x f + q\boldsymbol{\mathcal{E}}^{QC}[V, f] \cdot \nabla_p f = Q(f), \tag{4}$$

where we have included a collision operator $Q(f)$. The operator $Q(f)$ takes into account all the dissipative processes that affect the evolution of the particles in a media. Various scattering collision terms have been proposed. They can model particle-particle scattering and interaction of the particles with a background medium. e.g. electrons with phonons in a semiconductor lattice [3]. However, similarly to what happens in the classical case, in order to derive a fluid model it is not necessary to know all the details of collisions but only fairly general features, like for example, the conservation properties. Then, a reasonable and effective choice for the collisional term is the BGK operator

$$Q(f) = -\frac{1}{\tau}\left(f - \frac{\langle f \rangle}{\langle f_{\mathrm{eq}} \rangle} f_{\mathrm{eq}} \right),$$

where $\langle \cdot \rangle$ denotes integral with respect to $\mathbf{p}$, $\langle f \rangle = \frac{2}{(2\pi)^3} \int_{\mathbb{R}^3} f \, \mathrm{d}\mathbf{p}$, and f_{eq} is the equilibrium distribution function. We derive the equilibrium distribution function using the Maxwell and the Fermi-Dirac statistics. We introduce the function

$$F(t) = \begin{cases} \exp(-t) & \text{(Maxwell)} \\ \frac{1}{\exp(t)+1} & \text{(Fermi-Dirac)} \end{cases} \tag{5}$$

The equilibrium distribution function is given by

$$f_{\mathrm{eq}}(\mathbf{x}, \mathbf{p}) = F\left(\lambda_0^* + \frac{1}{2}\lambda_2^* \mathbf{p}^2 \right), \tag{6}$$

where λ_0^* is a function of $\mathbf{x}$ and of the external potential V, $\lambda_2^* = \frac{1}{mk_B T^*}$ depends on the constant equilibrium temperature T^*, with electron mass m and Boltzmann constant k_B. The function λ_0^* should be chosen to satisfy the equilibrium condition:

$$\frac{\mathbf{p}}{m} \cdot \nabla_x f_{\mathrm{eq}} + q\boldsymbol{\mathcal{E}}^{QC}[V, f_{\mathrm{eq}}] \cdot \nabla_p f_{\mathrm{eq}} = 0. \tag{7}$$

Thus, we find

$$\frac{k_B T^*}{q} \nabla_x \lambda_0^* + \boldsymbol{\mathcal{E}}^{QC}[V, f_{\mathrm{eq}}] = 0. \tag{8}$$

We will comment later on the quantum-corrected electric field $\boldsymbol{\mathcal{E}}^{QC}[V, f_{\mathrm{eq}}]$.

3 Hydrodynamic Limit

In this section, we derive the hydrodynamic limit of the previous equations. We make the following ansatz:

$$f(\mathbf{x},\mathbf{p},t)=F\left(\lambda_0+\boldsymbol{\lambda}_1\cdot\mathbf{p}+\frac{1}{2}\lambda_2\mathbf{p}^2\right), \tag{9}$$

with λ_0, $\boldsymbol{\lambda}_1$, λ_2 functions of $\mathbf{x}$, t, and F defined in (5). Equations for the λ's can be recovered by inserting the ansatz (9) in (4) and taking the moments with respect to the weights $(1,\mathbf{p}/m,\mathbf{p}^2/2m^2)$. We introduce the product $\langle f,g\rangle=\frac{2}{(2\pi)^3}\int_{\mathbb{R}^3} fg\,\mathrm{d}\mathbf{p}$. Using the identities:

$$\langle\nabla_p f,1\rangle=0,\qquad \left\langle\nabla_p f,\frac{\mathbf{p}}{m}\right\rangle=-\frac{1}{m}\langle f,1\rangle I,\qquad \left\langle\nabla_p f,\frac{\mathbf{p}^2}{2m^2}\right\rangle=-\frac{1}{m}\left\langle f,\frac{\mathbf{p}}{m}\right\rangle,$$

and noticing that $\boldsymbol{\mathcal{E}}^{QC}=\boldsymbol{\mathcal{E}}^{QC}[V,f]$ does not depend on $\mathbf{p}$, we find

$$\begin{cases}\dfrac{\partial}{\partial t}\langle f,1\rangle+\nabla_x\cdot\left\langle f,\dfrac{\mathbf{p}}{m}\right\rangle=\langle Q(f),1\rangle,\\[2ex]\dfrac{\partial}{\partial t}\left\langle f,\dfrac{\mathbf{p}}{m}\right\rangle+\nabla_x\cdot\left\langle f,\dfrac{\mathbf{p}}{m}\otimes\dfrac{\mathbf{p}}{m}\right\rangle-\dfrac{q}{m}\langle f,1\rangle\boldsymbol{\mathcal{E}}^{QC}=\left\langle Q(f),\dfrac{\mathbf{p}}{m}\right\rangle,\\[2ex]\dfrac{\partial}{\partial t}\left\langle f,\dfrac{\mathbf{p}^2}{2m^2}\right\rangle+\nabla_x\cdot\left\langle f,\dfrac{\mathbf{p}^2\mathbf{p}}{2m^3}\right\rangle-\dfrac{q}{m}\left\langle f,\dfrac{\mathbf{p}}{m}\right\rangle\cdot\boldsymbol{\mathcal{E}}^{QC}=\left\langle Q(f),\dfrac{\mathbf{p}^2}{2m^2}\right\rangle.\end{cases} \tag{10}$$

This is a system for the unknowns λ_0, $\boldsymbol{\lambda}_1$, λ_2. It is more convenient to write the evolution equations in terms of variables with a direct physical meaning. In analogy with the gas dynamics, we define

$$\lambda=\frac{1}{k_BTm\lambda_2}\left(\frac{\boldsymbol{\lambda}_1^2}{2\lambda_2}-\lambda_0\right),\quad \mathbf{v}=-\frac{\boldsymbol{\lambda}_1}{m\lambda_2},\quad T=\frac{1}{mk_B\lambda_2}, \tag{11}$$

which can be interpreted as the chemical potential divided by k_BT, the mean velocity and the temperature. The distribution function, both for Maxwell and Fermi-Dirac statistic, takes the form

$$f(\mathbf{x},\mathbf{p},t)=F\left(\frac{(\mathbf{p}-m\mathbf{v}(\mathbf{x},t))^2}{2mk_BT(\mathbf{x},t)}-\lambda(\mathbf{x},t)\right).$$

We introduce the function

$$\overset{\circ}{F}_\alpha(s)=\frac{1}{\Gamma(\alpha+1)}\int_0^\infty F(t-s)t^\alpha\,\mathrm{d}t,\quad \alpha\in\mathbb{R}, \tag{12}$$

which reduces to $\exp(s)$, for any α, for the Maxwell distribution, and to the complete Fermi-Dirac integral $F_\alpha(s)$, for the Fermi-Dirac distribution. It is possible to prove that

$$\overset{\circ}{F}{}'_\alpha(s)=\overset{\circ}{F}_{\alpha-1}(s).$$

We use $\overset{\circ}{F}_\alpha$ to get explicit relations for the number density n, the flux density $\mathbf{j}$ and the specific energy density e in terms of the variables λ, $\mathbf{v}$, T:

$$n=\langle f,1\rangle=n(\lambda,T), \tag{13}$$

$$\mathbf{j} = \left\langle f, \frac{\mathbf{p}}{m} \right\rangle = n(\lambda, T)\mathbf{v}, \tag{14}$$

$$e = \left\langle f, \frac{\mathbf{p}^2}{2m^2} \right\rangle = n(\lambda, T)\left(u(\lambda, T) + \frac{1}{2}\mathbf{v}^2\right), \tag{15}$$

with

$$n(\lambda, T) = n_0(T)\, \mathring{F}_{1/2}(\lambda), \quad n_0(T) = \frac{2(mk_BT)^{3/2}}{(2\pi)^{3/2}}, \tag{16}$$

$$u(\lambda, T) = \frac{3k_BT}{2m}\gamma_1(\lambda), \quad \gamma_1(\lambda) = \frac{\mathring{F}_{3/2}(\lambda)}{\mathring{F}_{1/2}(\lambda)}. \tag{17}$$

By substituting in (10) the following expressions

$$\left\langle f, \frac{\mathbf{p}}{m} \otimes \frac{\mathbf{p}}{m} \right\rangle = n(\lambda, T)\left(\frac{2}{3}u(\lambda, T)I + \mathbf{v} \otimes \mathbf{v}\right),$$

$$\left\langle f, \frac{\mathbf{p}^2}{2m^2}\frac{\mathbf{p}}{m} \right\rangle = n(\lambda, T)\left(\frac{5}{3}u(\lambda, T) + \frac{1}{2}\mathbf{v}^2\right)\mathbf{v},$$

$$\langle Q(f), 1 \rangle = 0,$$

$$\left\langle Q(f), \frac{\mathbf{p}}{m} \right\rangle = -\frac{1}{\tau}\mathbf{j},$$

$$\left\langle Q(f), \frac{\mathbf{p}^2}{2m^2} \right\rangle = -\frac{1}{\tau}n(\lambda, T)\left(u(\lambda, T) + \frac{1}{2}\mathbf{v}^2 - u\big(\lambda^*, T^*\big)\right),$$

with

$$\lambda^* = -\lambda_0^*, \qquad T^* = \frac{1}{mk_B\lambda_2^*}, \tag{18}$$

we obtain the system

$$\begin{cases} \dfrac{\partial n}{\partial t} + \nabla \cdot \mathbf{j} = 0, \\ \dfrac{\partial \mathbf{j}}{\partial t} + \nabla \cdot \left(\left(\dfrac{2}{3}e - \dfrac{\mathbf{j}^2}{3n}\right)I + \dfrac{1}{n}\mathbf{j} \otimes \mathbf{j}\right) - \dfrac{q}{m}n\boldsymbol{\mathcal{E}}^{QC} = -\dfrac{1}{\tau}\mathbf{j}, \\ \dfrac{\partial e}{\partial t} + \nabla \cdot \left(\left(\dfrac{5}{3}e - \dfrac{\mathbf{j}^2}{3n}\right)\dfrac{\mathbf{j}}{n}\right) - q\mathbf{j} \cdot \boldsymbol{\mathcal{E}}^{QC} = -\dfrac{1}{\tau}\big(e - nu^*\big). \end{cases} \tag{19}$$

The function $u^* = u(-\lambda_0^*, T^*)$ is obtained by solving the equilibrium Eq. (8) for a given external potential V, and by using Eq. (17). In particular, our model can be applied to systems for which the equilibrium temperature T^* is known from some physically based considerations. As an example, in the presence of the phonon thermal bath, the equilibrium temperature T^* equals the lattice temperature.

It is remarkable that the differential structure of this system is independent of the function F which we use to obtain the hydrodynamic limit. However, by means of (16), the specific choice of F does affect the reconstruction of the temperature and the chemical potential. In

fact, once we know n, $\mathbf{j}$ and e, we can find $u = \frac{e}{n} - \frac{\mathbf{j}^2}{2n^2}$, and thus solve (16), (17) for λ, T. More into details

Boltzmann statistic $F(t) = \exp(-t)$.

We have $\overset{\circ}{F}_\alpha(\lambda) = \exp(\lambda)$ for any α, so we find $\gamma_1(\lambda) = 1$, and

$$\lambda = \log\left(\frac{n}{n_0(T)}\right), \quad T = \frac{2mu}{3k_B}. \tag{20}$$

The temperature is proportional to the specific energy density.

Fermi-Dirac statistic $F(t) = (\exp(t) + 1)^{-1}$.

In this case $\overset{\circ}{F}_\alpha$ is the complete Fermi integral F_α, and we find

$$\lambda = F_{1/2}^{-1}\left(\frac{n}{n_0(T)}\right) = F_{3/2}^{-1}\left(\frac{n}{n_0(T)}\frac{2mu}{3k_BT}\right), \tag{21}$$

where the first equality gives λ and the second equality gives an equation which must be solved for T.

4 The Quantum-Corrected Electric Field

In this section, we analyze the behavior of the quantum corrected force $\boldsymbol{\mathcal{E}}^{QC}$ used in the fluid model. In particular, we show that the particle statistic distribution F plays the role of the smoothing function of the electric field.

The Fourier transform of the distribution function is given by

$$\widetilde{f}(\mathbf{x}, \boldsymbol{\eta}) = e^{-im\mathbf{v}\cdot\boldsymbol{\eta}} \int_{\mathbb{R}^3} F\left(\frac{\mathbf{p}^2}{2mk_BT} - \lambda\right) e^{-i\mathbf{p}\cdot\boldsymbol{\eta}}\, \mathrm{d}\mathbf{p} = e^{-im\mathbf{v}\cdot\boldsymbol{\eta}}\, \widetilde{f}_0(\mathbf{x}, \boldsymbol{\eta}),$$

with

$$f_0(\mathbf{x}, \mathbf{p}) = F\left(\frac{\mathbf{p}^2}{2mk_BT(\mathbf{x})} - \lambda(\mathbf{x})\right).$$

The function f_0 depends only by T and λ. We can make this dependence explicit by computing

$$\widetilde{f}_0 = \int_{\mathbb{R}^3} F\left(\frac{\mathbf{p}^2}{2mk_BT} - \lambda\right) e^{-i\mathbf{p}\cdot\boldsymbol{\eta}}\, \mathrm{d}\mathbf{p} = \frac{2\pi}{\eta} \int_0^\infty F\left(\frac{p^2}{2mk_BT} - \lambda\right) \sin(p\eta) 2p\, \mathrm{d}p,$$

with $p = |\mathbf{p}|$, $\eta = |\boldsymbol{\eta}|$. Expanding $\sin(p\eta)$ in power series of $p\eta$, and integrating by series, after some algebra we find

$$\widetilde{f}_0 = (2\pi mk_BT)^{3/2} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \left(\frac{mk_BT\eta^2}{2}\right)^k \overset{\circ}{F}_{k+1/2}(\lambda). \tag{22}$$

We can write this function in a more expressive way:

$$\widetilde{f}_0 = 4\pi^3 n(\lambda, T)\kappa(\eta, \lambda, T), \tag{23}$$

with

$$\kappa(\eta,\lambda,T)=\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\left(\frac{mk_BT\eta^2}{2}\right)^k\gamma_k(\lambda),\quad \gamma_k(\lambda)=\frac{\mathring{F}_{k+1/2}(\lambda)}{\mathring{F}_{1/2}(\lambda)}. \tag{24}$$

Then, Eq. (3) gives

$$\mathcal{E}_j^{QC}[V,f]=\mathcal{E}_j^{QC}[V,\lambda,T]=\frac{\int_{\mathbb{R}^3} i\eta_j\delta V(\mathbf{x},\boldsymbol{\eta})|\kappa(\eta,\lambda,T)|^2\,\mathrm{d}\boldsymbol{\eta}}{\int_{\mathbb{R}^3}\eta_j^2|\kappa(\eta,\lambda,T)|^2\,\mathrm{d}\boldsymbol{\eta}}. \tag{25}$$

For the Maxwell statistic, we have $\gamma_k=1$ for all k, and the function κ reduces to

$$\kappa(\eta,\lambda,T)=\kappa(\eta,T)=\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\left(\frac{mk_BT\eta^2}{2}\right)^k=\exp\left(-\frac{mk_BT\eta^2}{2}\right).$$

Then, we compute

$$\int_{\mathbb{R}^3}\eta_j^2\left|\kappa(\eta,T)\right|^2\mathrm{d}\boldsymbol{\eta}=\frac{\pi^{3/2}}{2(mk_BT)^{5/2}},$$

and we find the expression

$$\mathcal{E}_j^{QC}[V,T]=\frac{2(mk_BT)^{5/2}}{\pi^{3/2}}\int_{\mathbb{R}^3} i\eta_j\delta V(\mathbf{x},\boldsymbol{\eta})e^{-mk_BT\eta^2}\,\mathrm{d}\boldsymbol{\eta}, \tag{26}$$

which is independent of λ.

To understand the behavior of the electric field, we consider a one-dimensional system. The one-dimensional expression for the electric field can be obtained by assuming $V(\mathbf{x})=V(x)$, with $\mathbf{x}=(x,y,z)$, which leads to $\delta V(\mathbf{x},\boldsymbol{\eta})=\delta V(x,\eta)$, with $\boldsymbol{\eta}=(\eta,\xi,\zeta)$. Then,

$$\begin{aligned}\mathcal{E}_1^{QC}[V,T]&=\frac{2(mk_BT)^{5/2}}{\pi^{3/2}}\int_{\mathbb{R}^3} i\eta\delta V(x,\eta)e^{-mk_BT(\eta^2+\xi^2+\zeta^2)}\,\mathrm{d}\eta\,\mathrm{d}\xi\,\mathrm{d}\zeta\\&=-\frac{2(mk_BT)^{3/2}}{\hbar\pi^{1/2}}\int_{\mathbb{R}}\eta\left[V\left(x+\frac{\hbar}{2}\eta\right)-V\left(x-\frac{\hbar}{2}\eta\right)\right]e^{-mk_BT\eta^2}\,\mathrm{d}\eta,\\\mathcal{E}_2^{QC}[V,T]&=\mathcal{E}_3^{QC}[V,T]=0.\end{aligned}$$

In scaled variables, with

$$V_0=\frac{mx_0^2}{t_0^2},\qquad T_0=\frac{mx_0^2}{k_Bt_0^2},$$

we find

$$\mathcal{E}^{QC}=-\frac{2\Gamma^{3/2}}{\pi^{1/2}}T^{3/2}\int_{\mathbb{R}}\left[V\left(x+\frac{1}{2}\eta\right)-V\left(x-\frac{1}{2}\eta\right)\right]\eta e^{-\Gamma T\eta^2}\,\mathrm{d}\eta, \tag{27}$$

where we have introduced the dimensionless parameter

$$\Gamma=\left(\frac{mx_0^2}{\hbar t_0}\right)^2.$$

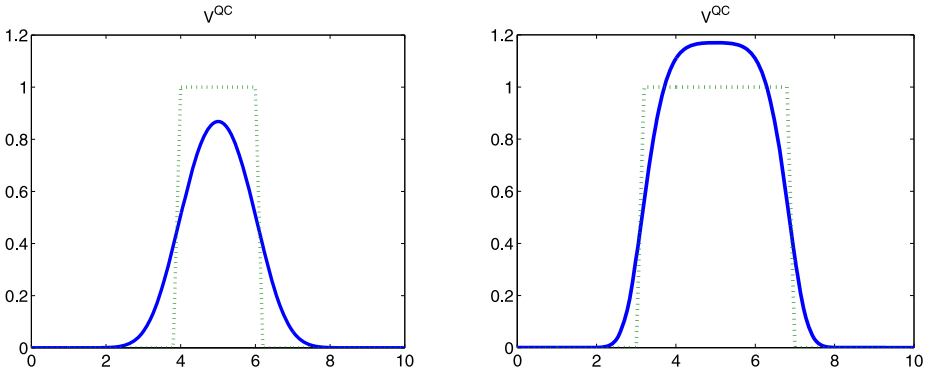

Fig. 1 Integrated quantum-corrected electric field (*continuous line*) and original electric potential (*dashed line*), for a thin (*left*) and a thick (*right*) potential barrier, with $\Gamma = 100$

In Fig. 1, we plot (in the equilibrium case) the integrated quantum-corrected electric field, which can be seen as a quantum-corrected electric potential, and compare it with the original potential V. One of the main characteristic of the quantum corrected potential is that it is typically smoother than the original bare potential. This has the considerable advantage to simplify the numerical treatment of the system avoiding the shocks experienced by the particles at the interface of the potential discontinuities. This behavior reflects the nonlocal nature of the quantum particles. As displayed in Fig. 1, the support of the quantum-corrected electric potential is larger than the support of the classical potential V. We can interpret this property by saying that the quantum particles "see" an effective potential obtained by the weighted average over few De Broglie wavelengths of the classical potential.

5 Extension

The approach followed in the previous sections is equivalent to solving a constrained maximization problem, assuming one knows the moments of the distribution function with respect to the weights $(1, \mathbf{p}, \mathbf{p}^2/2)$, for the entropy [8]

$$\mathcal{S} = \begin{cases} -\int_{\mathbb{R}^3} f(\log f - 1)\,\mathrm{d}\mathbf{p} & \text{(Maxwell)} \\ -\int_{\mathbb{R}^3} [f \log f + (1-f)\log(1-f)]\,\mathrm{d}\mathbf{p} & \text{(Fermi-Dirac)} \end{cases}$$

This approach can be extended to an arbitrary number of weights and corresponding moments. The main difference from the case presented in the previous sections is that, in general, the inversion of the constraints cannot be obtained explicitly. To show this, let us consider the weights $(1, \mathbf{p}, \frac{1}{2}\mathbf{p}^2, \frac{1}{2}\mathbf{p}^2\mathbf{p})$. The closure condition for the hydrodynamic evolution equations is obtained by imposing that the entropy $\mathcal{S}$ is maximized by f under the constraints

$$\begin{cases} \langle f, 1\rangle = n, & \left\langle f, \frac{1}{2}\mathbf{p}^2 \right\rangle = m^2 e, \\ \langle f, \mathbf{p}\rangle = m\mathbf{j}, & \left\langle f, \frac{1}{2}\mathbf{p}^2\mathbf{p} \right\rangle = m^3 \mathbf{j}_S. \end{cases} \tag{28}$$

They involve the number density n, the flux density $\mathbf{j}$, the specific energy density e and the specific energy flux density $\mathbf{j}_S$. This maximization problem leads to a distribution function of the form

$$f(\mathbf{x}, \mathbf{p}, t) = F\left(\lambda_0 + \boldsymbol{\lambda}_1 \cdot \mathbf{p} + \frac{1}{2}\lambda_2 \mathbf{p}^2 + \frac{1}{2}\mathbf{p}^2 \boldsymbol{\lambda}_3 \cdot \mathbf{p}\right), \tag{29}$$

where F is defined in (5), $\lambda_0, \boldsymbol{\lambda}_1, \lambda_2, \boldsymbol{\lambda}_3$ are Lagrange multipliers associated to the constraints (28) and are functions of $\mathbf{x}$, t. We note that the distribution function in (29) is well defined only in a bounded set of the momentum $\mathbf{p}$. This is the case, for example, of the electrons confined in a single band, where the momentum $\mathbf{p}$ is limited, by periodicity, to a bounded set. However, with this definition of distribution function is not possible to invert explicitly the constraints (28) and express the Lagrangian multipliers in terms of the basic moments. The inversion can be achieved by some approximations. We assume that the vector Lagrangian multipliers (with odd index) are small with respect to the isotropic multipliers (with even index) and we replace (29) with the approximate expression $f = f_0 + f_1$, where

$$f_0(\mathbf{x}, \mathbf{p}, t) = F\left(\lambda_0 + \frac{1}{2}\lambda_2 \mathbf{p}^2\right), \tag{30}$$

$$f_1(\mathbf{x}, \mathbf{p}, t) = F'\left(\lambda_0 + \frac{1}{2}\lambda_2 \mathbf{p}^2\right)\left(\boldsymbol{\lambda}_1 \cdot \mathbf{p} + \frac{1}{2}\mathbf{p}^2 \boldsymbol{\lambda}_3 \cdot \mathbf{p}\right). \tag{31}$$

The equations for the multipliers are obtained by inserting the previous ansatz in (4) and taking the moments with respect to the weights $(1, \mathbf{p}/m, \mathbf{p}^2/2m^2, \mathbf{p}^2\mathbf{p}/2m^2)$. We get the system (10) with one additional equation for the energy flux density:

$$\begin{aligned} &\frac{\partial}{\partial t}\left\langle f_1, \frac{\mathbf{p}^2 \mathbf{p}}{2m^3}\right\rangle + \nabla_x \cdot \left\langle f_0, \frac{\mathbf{p}^2}{2m^2}\frac{\mathbf{p}}{m} \otimes \frac{\mathbf{p}}{m}\right\rangle \\ &\quad - \frac{q}{m}\left\langle f_0, \frac{\mathbf{p}^2}{2m} I + \frac{\mathbf{p}}{m} \otimes \frac{\mathbf{p}}{m}\right\rangle \cdot \boldsymbol{\mathcal{E}}^{QC} = \left\langle Q(f), \frac{\mathbf{p}^2 \mathbf{p}}{2m^3}\right\rangle. \end{aligned} \tag{32}$$

We obtain

$$\begin{aligned} &n = \langle f_0, 1\rangle = n(\lambda, T), \qquad e = \left\langle f_0, \frac{\mathbf{p}^2}{2m^2}\right\rangle = n(\lambda, T) u(\lambda, T), \\ &\left\langle f_0, \frac{\mathbf{p}}{m} \otimes \frac{\mathbf{p}}{m}\right\rangle = \frac{2}{3} e I, \qquad \left\langle f_0, \frac{\mathbf{p}^2}{2m^2}\frac{\mathbf{p}}{m} \otimes \frac{\mathbf{p}}{m}\right\rangle = n\frac{5(k_B T)^2}{2m^2}\gamma_2(\lambda) I, \\ &\left\langle Q(f), \frac{\mathbf{p}^2 \mathbf{p}}{2m^3}\right\rangle = -\frac{1}{\tau}\mathbf{j}_S, \end{aligned}$$

and

$$\mathbf{j} = \left\langle f_1, \frac{\mathbf{p}}{m}\right\rangle = c_0 m \boldsymbol{\lambda}_1 + c_1 m^3 \boldsymbol{\lambda}_2, \qquad \mathbf{j}_S = \left\langle f_1, \frac{\mathbf{p}^2 \mathbf{p}}{2m^3}\right\rangle = c_1 m \boldsymbol{\lambda}_1 + c_2 m^3 \boldsymbol{\lambda}_2,$$

with $n(\lambda, T)$, $u(\lambda, T)$ given in (16), (17), and

$$c_i = \frac{2}{3}\left\langle F'\left(\lambda_0 + \frac{1}{2}\lambda_2 \mathbf{p}^2\right), \left(\frac{\mathbf{p}^2}{2m}\right)^{i+1}\right\rangle, \quad i = 0, 1, 2. \tag{33}$$

With this, we obtain the complete system:

$$\begin{cases} \dfrac{\partial}{\partial t} n + \nabla_x \cdot \mathbf{j} = 0, \\ \dfrac{\partial}{\partial t} \mathbf{j} + \nabla_x \left(\dfrac{2}{3} e \right) - \dfrac{q}{m} n \boldsymbol{\mathcal{E}}^{QC} = -\dfrac{1}{\tau} \mathbf{j}, \\ \dfrac{\partial}{\partial t} e + \nabla_x \cdot \mathbf{j}_S - \dfrac{q}{m} \mathbf{j} \cdot \boldsymbol{\mathcal{E}}^{QC} = -\dfrac{1}{\tau} \big(e - nu\big(\lambda^*, T^*\big) \big), \\ \dfrac{\partial}{\partial t} \mathbf{j}_S + \nabla_x \left(n \dfrac{5(k_B T)^2}{2m^2} \gamma_2(\lambda) \right) - \dfrac{5q}{3m} e \boldsymbol{\mathcal{E}}^{QC} = -\dfrac{1}{\tau} \mathbf{j}_S. \end{cases} \tag{34}$$

6 Conclusion

The derivation of a quantum-corrected hydrodynamic model for the out-of-equilibrium particle dynamics in the presence of particle collisions is presented. Our model is characterized by the presence of a quantum corrected electric force. This term depends nonlinearly to the particle distribution, current and energy. The advantage of this approach is that the modifications of the classical trajectories induced by the quantum mechanical nature of the particles, are taken into account by means of a smooth electric potential. This offers the considerable advantage that some quantum corrections can be easily included in a classical code. The modifications of the hydrodynamic equations for the Maxwell or the Fermi-Dirac statistic, are also discussed.

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