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Multiphase semiclassical approximation of an electron in a one-dimensional crystalline lattice – III. From ab initio models to WKB for Schrödinger–Poisson

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Dedicated to the memory of Frédéric Poupaud (1961–2004)

Abstract

This work is concerned with the semiclassical approximation of the Schrödinger–Poisson equation modeling ballistic transport in a 1D periodic potential by means of WKB techniques. It is derived by considering the mean-field limit of a N-body quantum problem, then K-multivalued solutions are adapted to the treatment of this weakly nonlinear system obtained after homogenization without taking into account for Pauli's exclusion principle. Numerical experiments display the behaviour of self-consistent wave packets and screening effects.

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1. Introduction

This article is the third and last part of a numerical study of semiclassical approximation of the motion of electrons in short-scale periodic potentials. We have now in mind to take into account also

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for the self-consistent interaction potential, which leads to a *weak nonlinearity*. More precisely, we are about to focus onto the following Schrödinger–Poisson equation in one space dimension

$$\mathrm{i}\hbar\partial_t\psi + \frac{\hbar^2}{2m}\partial_{xx}\psi = e(V_{\mathrm{ions}}(x) + V_{\mathrm{ext}}(x) + eV_{\mathrm{P}}(t,x))\psi, \quad -\epsilon_0\partial_{xx}V_{\mathrm{P}} = |\psi|^2; \ x \in \mathbb{R} \tag{1}$$

with $\hbar$ the Planck's constant, ϵ_0 the dielectric permittivity of the medium (it will be set to $\epsilon_0 \equiv 1$ throughout the whole paper), m and e the electronic mass and charge and $V_{\mathrm{ion}} \in \mathbb{R}$ the periodic potential modeling the interaction with a lattice of ionic cores. The smooth and slowly-varying external potential V_{ext} stands usually for an applied electric field, a confining potential or a doping term.

In order to shed complete light on the derivation and the qualitative properties of the simplified model (1), we first start from the exact Hamiltonian for a neutral system constituted of N atoms with Z electrons each in $\mathbb{R}^3$:

$$\mathbf{H} = \sum_{\alpha=1}^{N}\left\{\frac{\mathbf{P}_\alpha^2}{2M} + \sum_{i=1}^{Z}\frac{\mathbf{p}_{\alpha_i}^2}{2m} + \sum_{\beta(\neq\alpha)=1}^{N}\left[\frac{1}{2}\frac{(Ze)^2}{|\mathbf{X}_\alpha - \mathbf{X}_\beta|} + \sum_{i=1}^{Z}\left(-\frac{Ze^2}{|\mathbf{x}_{\beta_i} - \mathbf{X}_\alpha|} + \frac{1}{2}\sum_{j=1}^{Z}\frac{e^2}{|\mathbf{x}_{\alpha_i} - \mathbf{x}_{\beta_j}|}\right)\right]\right\}. \tag{2}$$

The notations have been chosen as follows: M, $\mathbf{P}_\alpha$, $\mathbf{X}_\alpha$ stand for the mass, momentum and position of the nuclei while $m, \mathbf{p}_{\alpha_i}, \mathbf{x}_{\alpha_i}$ refer to those of the electrons in the αth atom. All in all, this constitutes a system of $N(Z+1)$ charged particles interacting with each other via Coulombian forces (the atomic cores are lumped into a unique particle in this model). Ab initio computations will therefore refer to the ones involving this full Hamiltonian (2) which can be considered as exact in nonrelativistic quantum mechanics.

However, even for moderate values of N, Z, such ab initio computations become quickly almost impossible in terms of complexity. Hence, several simplifications are usually in order:

- The Born–Oppenheimer assumption states that the nuclei's motion decouples adiabatically because $M \gg m$; it can be neglected or at least treated classically.
- One can safely restrict (2) to vN valence and conduction electrons. All the others can generally be considered as tightly tied to the cores and confined inside the inner shells.

At this level, we have reduced our original system to a collection of N ions with v valence/conduction electrons. So the Hamiltonian (2) boils down to $\mathscr{H}_{\mathrm{ions}} + \mathscr{H}_{e^-}$ with

$$\mathscr{H}_{\mathrm{ions}} = \sum_{\alpha=1}^{N}\left\{\frac{\mathbf{P}_\alpha^2}{2M} + \frac{1}{2}\sum_{\beta(\neq\alpha)=1}^{N}\frac{(ve)^2}{|\mathbf{X}_\alpha - \mathbf{X}_\beta|}\right\}, \quad \mathscr{H}_{e^-} = \sum_{i=1}^{vN}\left\{\frac{\mathbf{p}_i^2}{2m} + V_{\mathrm{ions}}(\mathbf{x}_i) + \frac{1}{2}\sum_{j(\neq i)=1}^{vN}\frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|}\right\}. \tag{3}$$

The ionic potential $V_{\mathrm{ions}}(x) = \sum_{\alpha=1}^{N} V_{ps}(|x - X_\alpha|)$ where V_{ps} is a smoothered "pseudo-potential" originating from both Coulomb attraction and screening effects from inner shells electrons; it is referred to as the "effective core potential" in quantum chemistry. In the simplest Bohr–Oppenheimer framework, one assumes the $\mathbf{X}_\alpha$ to be constant and $\mathbf{P}_\alpha \equiv 0$ thus remains only $\mathscr{H}_{e^-}(\mathbf{x}, \mathbf{p})$ which can nonetheless constitute a delicate *quantum many-body problem*, especially in case $N \in \mathbb{N}$ is big.

A common way out lies in the *mean-field approximation* that we shall present in Section 2.1; roughly speaking, it consists in deriving self-consistently an average potential in place of the Coulomb interaction by letting $N \to \infty$ with a convenient scaling. Within this framework, electrons move as independent particles submitted to an overall mean electric field. The Pauli exclusion for fermions can be included or not in the derivation; Hartree or Hartree–Fock models are obtained accordingly. We shall choose to ignore it; hence we somehow consider an electron cloud treated as a *condensate*, that is a system endowed with the property that all its components share the *same one-particle state* described by a unique wave function

ψ solution of the Hartree equation.[1] This model as a "one-particle equation" is a somewhat crude approximation of the original many-body problem; since the wave function contributes to the effective potential only via its corresponding position density, this is the simplest realization of a *time-dependent density functional theory* (TDDFT). In the situation we consider in this article where (repulsive) Coulomb interaction is only to be taken into account, rigorous results have been obtained in case $V_{\text{ions}} \equiv 0$ in [5,6]. We shall indicate formally the changes that result from the inclusion of this potential. As the number of electrons is considered infinite, it is reasonable to assume that the number of corresponding ions diverges also; hence V_{ions} can be seen as a smooth *periodic* potential admitting a Bravais lattice endowed with a Wigner–Seitz cell in $\mathbb{R}^3$. This matches the physical setting of the articles [23,42,7,8].

We have in mind to conduct semiclassical computations on this Hartree model by means of the "two-scale WKB method" originally presented in [31] (see also [18,21,32]) extensively used in the linear setting (no self-interactions) in [28,26]. Relying on the well-known fact that the Hartree term is but the Green function of the Laplace operator in $\mathbb{R}^3$, we rewrite the mean-field equation as the weakly nonlinear Schrödinger–Poisson system. Then, assuming translational invariance in two independent space directions, [44], we move forward to a one-dimensional model like (1) (see [37,41,48] for examples of its physical realizations) to which it becomes possible to apply a variant of the linear WKB receipe. These derivations are presented in full detail within Section 2.2. Many (semi)classical limits have been carried out recently by means of the Wigner transform relying on the compactness lemma of [38]. In the context of the Schrödinger–Poisson system, it leads to a Vlasov–Poisson like equation possibly including the energy bands corresponding to the last valence or the first conduction levels; consult Section 2.3 and e.g. [38,7,50]. At a computational level, simulating measure solutions of this limit equation represents a heavy task even in one space dimension. Hence, we chosed to stick to the recent framework proposed by Brenier [15] (see also [1,12]) in Sections 3.1 and 3.2 for us to solve the Vlasov–Poisson problem in a mathematically simple but founded sense. It is then possible to use numerical techniques borrowed from [30] in order to update the intensities and thus the electric field in a semi-Lagrangian framework, see [10]. This is explained in detail in Section 3.3 assuming the reader familiar with the numerical techniques for K-branch solutions [16,24,25,28,26,27,46]. Other methodologies have been proposed in e.g. [20,22,34,35,39].

Section 4 is devoted to computational results. The first one is a self-consistent free electrons cloud's simulation; it corresponds somewhat to the simplest situation described by (1), namely $V'_{\text{ion}} \equiv 0$ and $V'_{\text{ext}} \equiv 0$, with initial data leading to a 5-branch solution thus asking for the inversion routines of [29]. Next, we take $V_{\text{ion}}(x) = \cos(x)$, the so-called Mathieu's potential already studied in [28,26]. At last, we tried to simulate the screening effect for an impurity in the same periodic potential, but with V_{ext} being a Coulomb term. For each of these, we expect to validate the proposed WKB algorithm against direct Schrödinger computations obtained via the Fourier schemes advocated in [3].

2. Hartree equation: mean-field assumption, WKB ansatz and Wigner analysis

2.1. Derivation of the Schrödinger–Poisson system via density functions

In this section, we aim at deriving the Hartree equation emanating from (3) within the strongest Born–Oppenheimer assumption, i.e., considering the ions steady. More precisely, we shall write down a "vN-body Schrödinger equation" (recall v as the number of valence/conduction electrons per atom) for the wave function $\Psi : \mathbb{R}^+ \times \mathbb{R}^{3vN} \to \mathbb{C}$ satisfying $i\hbar\partial_t \Psi = \mathscr{H}_{e^-}\Psi$. It would perhaps be more natural to consider a Hartree–Fock derivation instead, taking into account for the Pauli exclusion principle. However, recent numerical

[1] One speaks also about electrons (or mostly bosons) in *coherence*.

experiments suggest that for many physical situations, the parameters' size and the density are such that "exchange effects" can actually be neglected, see [4,43]. Thus, we first change to "atomic units" for which $\hbar = m = e = 1$ and without any loss of generality, we assume $v = 1$. Making explicit the dependence on $N \in \mathbb{N}$ of the wave function, there holds

$$\mathrm{i}\partial_t \Psi_N(t, \mathbf{x}_1, \ldots, \mathbf{x}_N) = -\frac{1}{2}\sum_{i=1}^{N}\{\Delta_{\mathbf{x}_i} + V_{\mathrm{ion}}(\mathbf{x}_i)\}\Psi_N + \frac{1}{N}\sum_{1\leqslant i<j\leqslant N} V_{\mathrm{Cou}}(|\mathbf{x}_j - \mathbf{x}_i|)\Psi_N, \tag{4}$$

with $\mathbf{x}_i \in \mathbb{R}^3$ and V_{Cou} standing for the Coulomb term, already studied in the semiclassical context in [26], Section 5. We also introduce the density, $D_N(t, \mathbf{X}_N, \mathbf{Y}_N) = \Psi_N(t, \mathbf{X}_N)\overline{\Psi_N(t, \mathbf{Y}_N)} \in \mathbb{C}$, where $\mathbf{X}_N = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$ and $\mathbf{Y}_N = (\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_N) \in \mathbb{R}^{3N}$. At this level, it is convenient to define another important object, namely its nth *marginal* for any $\mathbb{N} \ni n < N$:

$$D_{N:\,n}(t, \mathbf{x}_1, \ldots, \mathbf{x}_n, \mathbf{y}_1, \ldots, \mathbf{y}_n) = \int_{\mathbb{R}^{3(N-n)}} D_N(t, \mathbf{x}_1, \ldots, \mathbf{x}_n, z_{n+1}, \ldots, z_N, \mathbf{y}_1, \ldots, \mathbf{y}_n, z_{n+1}, \ldots, z_N)\mathrm{d}z_{n+1}, \ldots, \mathrm{d}z_N.$$

One observes at once that the *local position density* $\varrho(t, \mathbf{x})$ reads: $\varrho(t, \mathbf{x}) = D_{N:1}(t, \mathbf{x}, \mathbf{x})$ for any $\mathbf{x} \in \mathbb{R}^3$. All these quantities can be deduced from Eq. (4). It is now that the "coherence assumption" comes into play since we must complete (4) with peculiar initial data like

$$\Psi_N(t = 0, \mathbf{x}_1, \ldots, \mathbf{x}_N) = \prod_{i=1}^{N}\psi_0(\mathbf{x}_i), \tag{5}$$

which expresses the fact that initially, all the N electrons located in $\mathbf{x}_{i=1,\ldots,N}$ are in the same quantum state ψ_0, an assumption which violates Pauli's exclusion principle.[2] Nevertheless, the idea is to prove, at least formally, that this "ansatz" propagates in time $t \in \mathbb{R}^+$ asymptotically in $N \to \infty$.

It is well-known that densities satisfy the Von-Neumann equation

$$\begin{aligned}\mathrm{i}\partial_t D_N(t, \mathbf{X}_N, \mathbf{Y}_N) = &-\frac{1}{2}[\Delta_{\mathbf{X}_N} - \Delta_{\mathbf{Y}_N}]D_N(t, \mathbf{X}_N, \mathbf{Y}_N) + \sum_{i=1}^{N}[V_{\mathrm{ion}}(\mathbf{x}_i) - V_{\mathrm{ion}}(\mathbf{y}_i)]D_N(t, \mathbf{X}_N, \mathbf{Y}_N)\\ &+\frac{1}{N}\sum_{1\leqslant i<j\leqslant N}[V_{\mathrm{Cou}}(|\mathbf{x}_j - \mathbf{x}_i|) - V_{\mathrm{Cou}}(|\mathbf{y}_j - \mathbf{y}_i|)]D_N(t, \mathbf{X}_N, \mathbf{Y}_N)\end{aligned}$$

from where one deduces the BBGYK[3] hierarchy for each of the nth marginals [6]:

$$\begin{aligned}\mathrm{i}\partial_t D_{N:\,n}(t, \mathbf{X}_n, \mathbf{Y}_n) = &-\frac{1}{2}[\Delta_{\mathbf{X}_n} - \Delta_{\mathbf{Y}_n}]D_{N:\,n}(t, \mathbf{X}_n, \mathbf{Y}_n)\\ &+\sum_{i=1}^{n}\int_{\mathbb{R}^{3(N-n)}}[V_{\mathrm{Cou}}(|\mathbf{x}_i - z|) - V_{\mathrm{Cou}}(|\mathbf{y}_i - z|)]D_{N:\,n+1}(t, \mathbf{X}_n, z, \mathbf{Y}_n, z)\cdot \mathrm{d}z\\ &+e(n, N) + \sum_{i=1}^{n}[V_{\mathrm{ion}}(\mathbf{x}_i) - V_{\mathrm{ion}}(\mathbf{y}_i)]D_{N:\,n}(t, \mathbf{X}_n, \mathbf{Y}_n),\end{aligned} \tag{6}$$

since the last integral term coming from V_{ion} vanishes identically; $e(n, N)$ stands for an error term going to zero as $N \to +\infty$.

Now, it is tempting to consider the "self-consistent one-particle equation":

$$\mathrm{i}\partial_t \psi = -\frac{1}{2}\Delta_{\mathbf{x}}\psi + V_{\mathrm{ion}}(\mathbf{x})\psi + \left(\int_{\mathbb{R}^3} V_{\mathrm{Cou}}(|\mathbf{x} - z|)|\psi(t, z)|^2 \cdot \mathrm{d}z\right)\psi, \tag{7}$$

[2] A Slater determinant [2], could be considered instead.
[3] After Born, Bogolyubov, Green, Yvon and Kirkwood.

for which the density reads simply $\rho(t,\mathbf{x},\mathbf{y}) = \psi(t,\mathbf{x})\overline{\psi(t,\mathbf{y})}$ for $\mathbf{x}$, $\mathbf{y}$ in $\mathbb{R}^3$. The same way, it can be shown to solve a "one-particle Von-Neumann equation",

$$\mathrm{i}\partial_t\rho(t,\mathbf{x},\mathbf{y}) = -\frac{1}{2}[\Delta_{\mathbf{x}} - \Delta_{\mathbf{y}}]\rho(t,\mathbf{x},\mathbf{y}) + [V_{\mathrm{ion}}(\mathbf{x}) - V_{\mathrm{ion}}(\mathbf{y})]\rho(t,\mathbf{x},\mathbf{y}) + \rho(t,\mathbf{x},\mathbf{y})\left(\int_{\mathbb{R}^3}[V_{\mathrm{Cou}}(|\mathbf{x}-z|) - V_{\mathrm{Cou}}(|\mathbf{y}-z|)]\rho(t,z,z)\cdot \mathrm{d}z\right),$$

from which we infer that $\rho_n(t,\mathbf{X}_n,\mathbf{Y}_n) \overset{\mathrm{def}}{=} \prod_{i=1}^n \rho(t,\mathbf{x}_i,\mathbf{y}_i)$ is solution of an infinite hierarchy similar to (6):

$$\mathrm{i}\partial_t\rho_n(t,\mathbf{X}_n,\mathbf{Y}_n) = -\frac{1}{2}[\Delta_{\mathbf{X}_n} - \Delta_{\mathbf{Y}_n}]\rho_n(t,\mathbf{X}_n,\mathbf{Y}_n) + \sum_{i=1}^n [V_{\mathrm{ion}}(\mathbf{x}_i) - V_{\mathrm{ion}}(\mathbf{y}_i)]\rho_n(t,\mathbf{X}_n,\mathbf{Y}_n) + \sum_{i=1}^n \int_{\mathbb{R}^{3(N-n)}} [V_{\mathrm{Cou}}(|\mathbf{x}_i - z|) - V_{\mathrm{Cou}}(|\mathbf{y}_i - z|)]\rho_{n+1}(t,\mathbf{X}_n,z,\mathbf{Y}_n,z)\cdot \mathrm{d}z.$$

Hence, it is reasonable to expect that under the same hypotheses as in [5], i.e. $\psi_0 \in H^2(\mathbb{R}^3)$ and (5), the following convergence holds:

$$\forall t \in \mathbb{R}^+, \quad (\mathbf{x},\mathbf{y}) \in \mathbb{R}^6, \quad D_{N:\,1}(t,\mathbf{x},\mathbf{y}) \overset{N\to\infty}{\to} \rho(t,\mathbf{x},\mathbf{y}).$$

By a uniqueness result for the Cauchy problem on the infinite hierarchies [5], this implies that ψ solution of (7) is related to (4) via $\Psi_N(t,\mathbf{x}_1,\ldots,\mathbf{x}_N) = \prod_{i=1}^N \psi(t,\mathbf{x}_i)$, up to an error that goes eventually to zero as $N \to \infty$. This expresses the fact that electrons remain in coherence as time increases. All in all, mean-field provides a convenient way to compute approximately a global wave function Ψ_N solution of (4) from the knowledge of a simpler one ψ solving the self-consistent problem (7); this shortcut is only meant to be relevant for large values of $N \in \mathbb{N}$. The final step is to rewrite (7) as

$$\mathrm{i}\partial_t\psi(t,\mathbf{x}) = -\frac{1}{2}\Delta_{\mathbf{x}}\psi(t,\mathbf{x}) + V_{\mathrm{ion}}\psi(t,\mathbf{x}) + V_{\mathrm{P}}(t,\mathbf{x})\psi(t,\mathbf{x}), \tag{8}$$

where the self-consistent potential $V_P = V_{\mathrm{Cou}} *_{\mathbf{x}} |\psi|^2$, which is equivalent to say that V_{P} solves the Poisson equation:

$$-\Delta_{\mathbf{x}} V_{\mathrm{P}}(t,\mathbf{x}) = |\psi|^2(t,\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3. \tag{9}$$

If we restrict ourselves to models endowed with translational invariance in 2 space dimensions [44], a one-dimensional problem like (1) arises. The preceding derivation seems to indicate that only smooth initial data $\psi(t=0,.) = \psi_0 \in H^2(\mathbb{R}^3)$ are relevant, like in [5].

2.2. Bloch spectrum and the one-dimensional (linear) WKB ansatz

From the former section, one can notice that the mean-field model (7) is mostly concerned with a "large system" containing an infinite number of *strongly delocalized* valence/conduction electrons which wander inside the material. A concrete example of such a system is given by a *metal cluster*, see [13], where N can grow from 1000 up to the Avogadro's number (which may be considered as "infinite" in practice). Typically, mean-field is too much of a rough approximation for quantum chemistry. Relying on these considerations, it is quite natural to switch to the characteristic scales of the bulk system under consideration; thus a dimensionless parameter ε is introduced, which measures the microscopic–macroscopic ratio. We can assume it small in order to look for "wave-packet solutions" of (7) with a spatial spreading of the order of $1/\varepsilon$. Physically speaking, this means *exactly* that only strongly delocalized electrons wandering inside the crystal are sought.

Sticking hereafter to our one-dimensional model, we recast (1) in macroscopic variables $x \mapsto x/\varepsilon$, $t \mapsto t/\varepsilon$ and taking into account for the slowly-varying exterior potential V_{ext}, we obtain a scaled problem as in [28,26],

$$\mathrm{i}\varepsilon\partial_t\psi + \frac{\varepsilon^2}{2}\partial_{xx}\psi = V_{\text{ion}}\left(\frac{x}{\varepsilon}\right)\psi + (V_{\text{P}}\psi) + V_{\text{ext}}(x)\psi, \quad V_{\text{ion}}(x+2\pi) = V_{\text{ion}}(x), \tag{10}$$

for which V_{P} stands for the self-consistent potential and V_{ext} is smooth and independent of time. From now on, we assume the lattice period to be 2π on the atomic lengthscale for the sake of simplicity only.

The naive "WKB plane-wave" ansatz $A(t,x)\exp(\mathrm{i}\varphi(t,x)/\varepsilon)$ doesn't have the correct structure hence following [18,21,31], we shall consider instead a two-scale amplitude $A(t,x,x/\varepsilon)\exp(\mathrm{i}\varphi(t,x)/\varepsilon)$ as follows:

$$A\left(t,x,y=\frac{x}{\varepsilon}\right) = A_0(t,x,y) + \varepsilon A_1(t,x,y) + \cdots; \quad A(t,x,y+2\pi) = A(t,x,y) \in \mathbb{C}. \tag{11}$$

Since we are interested in arbitrary small values of $\varepsilon \geqslant 0$, the $x \in \mathbb{R}$ and $y \in \mathbb{R}$ variables must be uncorrelated. Taking this new dependence into account inside (10) yields the expression:

$$\begin{aligned} &-A\partial_t\varphi + \frac{1}{2}(\partial_{yy}A - A(\partial_x\varphi)^2 + 2\mathrm{i}(\partial_x\varphi)(\partial_y A)) - (V_{\text{ion}}(y) + V_{\text{ext}}(x) + V_{\text{P}}(t,x))A \\ &\quad + \frac{\mathrm{i}\varepsilon}{2}(2\partial_t A + A\partial_{xx}\varphi + 2\partial_x A\ \partial_x\varphi - 2\mathrm{i}\partial_{xy}A) + \frac{\varepsilon^2}{2}\partial_{xx}A = 0. \end{aligned} \tag{12}$$

- The O(1) terms inside (12) rewrite

$$-\left\{(\partial_t\varphi + V_{\text{ext}}(x) + V_{\text{P}}(t,x)) - \left(\frac{1}{2}(\partial_y + i(\partial_x\varphi))^2 - V_{\text{ion}}(y)\right)\right\}A,$$

thus they cancel if and only if $y \mapsto A_0(t,x,y)\exp(\mathrm{i}\kappa y)$ is an eigenstate of $\mathscr{H}(\hat{p},y) = -\frac{1}{2}\partial_{yy} + V_{\text{ion}}(y)$, $\hat{p} = i\partial_y$, written in Bloch wave form, see [11,45] and associated to the eigenvalue $E(\partial_x\varphi) = -\partial_t\varphi - V_{\text{ext}}(x) - V_{\text{P}}(t,x)$:

$$\mathscr{H}(y,\hat{p})(A_0\exp(\mathrm{i}\kappa y)) = -(\partial_t\varphi + V_{\text{ext}}(x) + V_{\text{P}}(t,x))\ (A_0\exp(\mathrm{i}\kappa y)), \quad \kappa = \partial_x\varphi.$$

That is to say, we want $y \mapsto \Psi_\kappa(y) = \exp(\mathrm{i}\kappa y)A_0(t,x,y)$ to satisfy for all $(t,x) \in \mathbb{R}^+ \times \mathbb{R}$:

$$\forall y \in \mathbb{R}, \quad \mathscr{H}(\hat{p},y)\Psi_\kappa = -\frac{1}{2}\partial_{yy}\Psi_\kappa + V_{\text{ion}}(y)\Psi_\kappa = E(\kappa)\Psi_\kappa. \tag{13}$$

Note that the slow variable x shows up only as a parameter; thus an Hamilton–Jacobi equation has been derived from this cell problem

$$\partial_t\varphi + E(\partial_x\varphi) + V_{\text{ext}}(x) + V_{\text{P}}(t,x) = 0. \tag{14}$$

However, it isn't clear at this level why the Poisson potential doesn't depend on the fast scale $y = x/\varepsilon$ as A_0 does.

- The second step consists in writing $A_0(t,x,y) = a_0(t,x)z_\kappa(y)$ with stationary 2π-periodic orthonormal modulations: $\|z_\kappa\|_{L^2(0,2\pi)} = 1$. Then following [18], the solvability condition to make $\mathrm{O}(\varepsilon)$ remainder terms in (12) vanish leads to the modified transport equation:

$$\partial_t a_0 + E'(\partial_x\varphi)\partial_x a_0 + \frac{a_0}{2}\partial_x E'(\partial_x\varphi) + \beta(t,x)a_0 = 0. \tag{15}$$

The phase-shift term is purely imaginary; $\beta(t,x) = \mathrm{i}\Im\beta(t,x)$ ($\Im$. standing for the imaginary part of a complex number). It is sometimes referred to as the *Berry phase* which stems from the interaction between the periodic lattice and the exterior potentials. However, one can always multiply (15) by $2\bar{a}_0$ and take its real part in order to derive the more usual continuity equation for the intensity $|a_0|^2$:

$$\partial_t |a_0|^2 + \partial_x (|a_0|^2 \, E'(\partial_x \varphi)) = 0. \tag{16}$$

- We must at last indicate how to extract the Poisson potential V_P from φ, Ψ_κ and the principal amplitude a_0. The computation is shown for the pre-caustic region, and for a smooth wave-function ψ (we recall from Section 2.1 that presumably, $\psi_0 \in H^2(\mathbb{R})$). Let us start from

$$-\partial_{xx} V_P(t,x) = |\psi|^2(t,x) = |a_0(t,x)|^2 |z_\kappa(x/\varepsilon)|^2, \quad \kappa = \partial_x \varphi.$$

Since $y \mapsto z_\kappa(y)$ is 2π-periodic and C^∞ (energy bands are isolated in 1d, see e.g., the introduction of [8]), it can be written as its Fourier series:

$$\begin{aligned} -V_P(t,x) &= \int^x \int^{x'} |a_0(t,s)|^2 |z_{\kappa(t,s)}(s/\varepsilon)|^2 \cdot \mathrm{d}s \cdot \mathrm{d}x' \\ &= \sum_{j,j' \in \mathbb{Z}} \int^x \int^{x'} \left\{ (a_0 \cdot \overline{a_0})(t,s) \hat{z}_\kappa^j \cdot \overline{\hat{z}_\kappa^{j'}} \right\} \exp(\mathrm{i}(j-j')s/\varepsilon) \cdot \mathrm{d}s \cdot \mathrm{d}x'. \end{aligned}$$

This self-consistent potential is defined up to 2 constants coming from boundary/decay conditions for the Poisson equation. We now integrate by parts making use of $\exp(\mathrm{i}(j-j')s/\varepsilon) = \frac{-\mathrm{i}\varepsilon}{j-j'} \partial_s \{\exp(\mathrm{i}(j-j')s/\varepsilon)\}$ and the smoothness of a_0 and z_κ. The terms $j = j'$ yield an adiabatic decoupling:

$$-V_P(t,x) = \int^x \int^{x'} |a_0(t,s)|^2 \underbrace{\|z_{\kappa(t,s)}(\cdot)\|^2_{L^2(0,2\pi)}}_{\sum_{j \in \mathbb{Z}} |\hat{z}_\kappa^j|^2 = 1} \cdot \mathrm{d}s \cdot \mathrm{d}x' + \mathrm{O}(\varepsilon^m), \tag{17}$$

where $m \in \mathbb{N}$ is the smoothness of a_0, i.e., $x \mapsto a_0(t,x)$ is of class C^m for t in some time interval. This is somewhat a homogenization process for the Poisson equation arising in this 1d context. In a 3-D case, a stationary phase argument on the Hartree term would (formally) give a similar result with $m = 1$ (see also [19,40]).

All in all, starting from the Schrödinger equation (10), one has to consider the Bloch spectral decomposition (13) producing a countable set of distorted plane waves Ψ_κ^n, $n \in \mathbb{N}$, associated to the energy bands $E_n(\kappa)$; consult [2,7,11,18,21,31,28,26,42] for more details. Thus a convenient nth band ansatz reads (as in the linear case) at least before breakup,

$$\psi_n^\varepsilon(t,x) = a_0(t,x) \exp\left(\frac{\mathrm{i}\varphi(t,x)}{\varepsilon}\right) z_\kappa^n(x/\varepsilon), \quad \kappa = \partial_x \varphi(t,x), \tag{18}$$

where the unknowns evolve according to the nth band *weakly nonlinear* WKB system:

$$\partial_t \varphi + E_n(\partial_x \varphi) + V_{\mathrm{ext}}(x) + V_P(t,x) = 0, \quad \partial_t \mu + \partial_x (E_n'(\partial_x \varphi) \; \mu) = 0, \quad -\partial_{xx} V_P(t,x) = \mu = |a_0|^2. \tag{19}$$

Eqs. (18) and (19) mean in particular that an initial datum in the nth band $E_n(\kappa)$, z_κ^n always leads to an approximate solution in the same band; hence the Poisson nonlinearity induces a behaviour not so different compared to the linear cases in [26]. This is one of the reasons why it is possible to extend K-branch solutions to cover the present situation.

Remark 1. The post-caustic region is more delicate to handle as we expect $\varphi$and μ to become multivalued as in [28,26]. So, in order to remain consistent, the Poisson equation will involve $\mu_{1,2,\ldots}$, plus many cross-terms which go weakly to zero (as formally shown in [28] Section 3.2) except on caustics and at the edges of the Brillouin zone. Hence another $\mathrm{O}(\varepsilon)$ error term comes into play when neglecting them. We shall go back to that in Section 4.

2.3. Rigorous semiclassical limit: the Wigner–Bloch series

In this section, we shall recall briefly the main result from [7] concerning the semiclassical behaviour of mixed-states for (8) and (9), in our 1D context (10) though. More precisely, we consider a scaled system of equations in $\mathbb{R}^+ \times \mathbb{R}$

$$\begin{aligned} &i\varepsilon\partial_t\psi_j^\varepsilon + \frac{\varepsilon^2}{2}\partial_{xx}\psi_j^\varepsilon = V_{\text{ion}}\left(\frac{x}{\varepsilon}\right)\psi_j^\varepsilon + (V_{\text{P}}^\varepsilon\psi_j^\varepsilon), \quad V_{\text{ion}}(x+2\pi) = V_{\text{ion}}(x), \psi_j^\varepsilon(t=0,x) = \psi_{j,0}^\varepsilon(x), \ \ j \in \mathbb{N}, \\ &\varrho^\varepsilon(t,x) = \sum_{j\in\mathbb{N}} \lambda_j^\varepsilon |\psi_j^\varepsilon(t,x)|^2; \quad -\partial_{xx}V_{\text{P}}^\varepsilon = \varrho^\varepsilon. \end{aligned} \tag{20}$$

The infinite vector $(\psi_j^\varepsilon)_{j\in\mathbb{N}}$ represents the quantum mixed state of the system under consideration. Furthermore, it is assumed:

$$\lambda_j^\varepsilon \geqslant 0, \quad \sum_{j\in\mathbb{N}} \lambda_j^\varepsilon = 1, \quad \sum_{j\in\mathbb{N}} (\lambda_j^\varepsilon)^2 \leqslant O(1)\varepsilon^3.$$

Then, from the Bloch decomposition recalled in Section 2.2, one defines the *Wigner–Bloch series* as follows,

$$w_n^\varepsilon(t,x,\xi) = \sum_{\gamma\in 2\pi\mathbb{Z}} \zeta_{n,n}^\varepsilon\left(x + \frac{\varepsilon}{2}\gamma, x - \frac{\varepsilon}{2}\gamma\right)\exp(-i\gamma\xi),$$

with $\zeta_{n,p}^\varepsilon$ standing for the Bloch density matrix built from the projectors $\mathscr{I}_n^\epsilon$ onto the wave-packet subspaces $\mathscr{S}_n^\epsilon$ (notation borowed from [28], Section 2.3 is used here),

$$\forall x,y \in \mathbb{R}^2, \quad \zeta_{n,p}^\varepsilon(t,x,y) = \sum_{j\in\mathbb{N}} \lambda_j^\varepsilon \mathscr{I}_n^\epsilon\psi_j^\varepsilon(t,x)\overline{\mathscr{I}_p^\varepsilon\psi_j^\varepsilon(t,y)}.$$

Now, let the initial data concentrate inside an isolated energy band $E_n(\kappa)$, like e.g., (18), then it follows that, in convenient topologies,

$$w_n^\varepsilon(t,x,\xi) \overset{\varepsilon\to 0}{\rightharpoonup} f(t,x,\xi) \geqslant 0, \quad \varrho^\varepsilon(t,x) \overset{\varepsilon\to 0}{\rightharpoonup} \varrho(t,x) := \int_{-\frac{1}{2}}^{\frac{1}{2}} f(t,x,\xi)\cdot d\xi, \quad V_{\text{P}}^\varepsilon \to V_{\text{P}}.$$

Moreover, the kinetic distribution f satisfies the semiclassical (nth band) Vlasov–Poisson equation

$$\partial_t f + E_n'(\xi)\partial_x f - \partial_x V_{\text{P}}(t,x)\partial_\xi f = 0, \quad -\partial_{xx}V_{\text{P}} = \varrho, \tag{21}$$

in the sense of distributions. One sees here one big advantage in using WKB methods in the present context when compared to Wigner techniques. Indeed, WKB construction delivers a rather simple expression (18) for a wave function belonging to the nth energy band and approximately satisfying (1) for $t \geqslant 0$ and ε positive but small enough through the solving of (19). In sharp constrast, Wigner techniques furnish only information on the ideal $\varepsilon = 0$ case discarding fine-scale modulations $z_\kappa^n(\cdot/\varepsilon)$; it would therefore be more difficult to study numerically the weak consistency of physical observables relying on this approach, left apart the more singular moment systems admitting measure-valued solutions, see [27,33,46,49]. However, results of this type do provide a guideline as we shall see in the forthcoming section.

3. K-branch solutions with a weak nonlinearity

K-branch solutions, see e.g. [14,16,24,25,46], have been used up to now exclusively in the context of *linear* dispersive equations. Hence, we must show now how to adapt this tool in order to tackle the weakly nonlinear problem (19).

3.1. Lagrangian solutions for Vlasov–Poisson in 1D with $V'_{\mathrm{ext}} \equiv 0$

The Hamilton–Jacobi equation in (19) must be considered in a "geometric sense", i.e., relying on the method of characteristics. We also want our framework to be fully consistent with the "ideal case" $\varepsilon = 0$ studied in [7,44,50] by means of Bloch–Wigner series where a (nth band) Vlasov–Poisson equation is derived

$$\partial_t f + \partial_x(E_n'(\xi)f) + \partial_\xi(F(t,x)f) = 0, \quad f(t=0,x,\xi) = f_0(x,\xi) \tag{22}$$

and where $F(t,x)$ stands for the electric field $F = -\partial_x V_{\mathrm{P}}$. We aim at building solutions by means of a method which can easily be implemented on a computer. So, following a recent paper by Brenier [15], we start with a N-particle density function,

$$f_N(t,x,\xi) = \frac{1}{N}\sum_{\alpha=1}^{N} \delta(x - X_\alpha(t))\delta(\xi - U_\alpha(t)), \quad t \geqslant 0,$$

$\delta(\cdot)$ the Dirac measure in 0, which evolves according to the differential system:

$$\dot{X}_\alpha(t) = E_n'(U_\alpha)(t), \quad \dot{U}_\alpha(t) = F(t, X_\alpha(t)). \tag{23}$$

The trick is based on the fact that the Laplacian's Green function in 1d is but the Heaviside function H; accordingly,

$$\partial_x F(t,x) = \int_{\mathbb{R}} f_N(t,x,\xi)\cdot \mathrm{d}\xi = \frac{1}{N}\sum_{\alpha=1}^{N}\delta(x - X_\alpha(t)),$$

which yields:

$$F(t,x) = \frac{1}{N}\sum_{\alpha=1}^{N} H(x - X_\alpha(t)), \quad H(0) = \frac{1}{2}. \tag{24}$$

From [12,15], we know that the nonlinear differential system (23) and (24) is well-posed in phase-space for any value $N \in \mathbb{N}$ thus we get:

$$\dot{X}_\alpha(t) = E_n'(U_\alpha)(t), \quad \dot{U}_\alpha(t) = \frac{1}{N}\sum_{\beta=1}^{N} H(X_\alpha(t) - X_\beta(t)).$$

We stress that, since $N \in \mathbb{N}$ is finite, this is but a $2N \times 2N$ autonomous first-order differential system with a BV right-hand side. So the associated Liouville equation is *linear* and the renormalization property of [12] fully applies hence ensures well-posedness. However, we now intend to pass *formally* to the continuous limit $N \to \infty$ hence $f(t,x,\xi) = \int_{\mathbb{R}}\delta(x - X(t,\alpha))\delta(\xi - U(t,\alpha))\cdot \mathrm{d}\alpha$ for which (23) and (24) boils down to:

$$\partial_t X(t,\alpha) = E_n'(U(t,\alpha)), \qquad \partial_t U(t,\alpha) = \int_0^R H(X(t,\alpha) - X(t,\alpha'))\cdot \mathrm{d}\alpha', \tag{25}$$

where $R = \|a_0(t=0,.)\|^2_{L^2(\mathbb{R})}$. This is a one-dimensional bicharacteristics system for the semiclassical Vlasov-Poisson equation and we shall interpret (19) in this "geometric sense" hereafter, (see also Remark IV.6 in [38]). Of course, the symbol α which refers to the Lagrangian mass variable has here a completely different meaning compared to [43].

Let us now show that this (Lagrangian) construction is consistent with (22):

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^2} f(t,x,\xi)\phi(x,\xi)\cdot \mathrm{d}x\cdot \mathrm{d}\xi &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}} \phi(X(t,\alpha),U(t,\alpha))\cdot \mathrm{d}\alpha\\ &= \int_{\mathbb{R}} \{\partial_x\phi(X,U)\partial_t X + \partial_\xi\phi(X,U)\partial_t U\}(t,\alpha)\cdot \mathrm{d}\alpha\\ &= \int_{\mathbb{R}} \{\partial_x\phi(X,U)E_n'(U(t,\alpha)) + \partial_\xi\phi(X,U)F(t,X(t,\alpha))\}\cdot \mathrm{d}\alpha\\ &= \int_{\mathbb{R}} f(t,x,\xi)\{\partial_x\phi(x,\xi)E_n'(\xi) + \partial_\xi\phi(x,\xi)F(t,x)\}\cdot \mathrm{d}x\cdot \mathrm{d}\xi.\end{aligned}$$

The third step uses the definition of the differential system (25) and the last one is just a consequence of the definition of f by means of Dirac masses. So clearly we have derived a weak formulation of (22) for any test function $\phi \in C^1(\mathbb{R}^2)$. At last, the case $V'_{\mathrm{ext}} \neq 0$ can be handled by replacing $F(t, X_\alpha(t))$ by $F(t,X_\alpha(t)) - V'_{\mathrm{ext}}(X_\alpha(t))$ in (23) and so on.

3.2. Consistency of bicharacteristics' system (25) before breakup

We shall consider monokinetic initial data, like in [50]

$$f(t=0,x,\xi) = \varrho_0(x)\delta(\xi - u_0(x)), \quad \varrho_0 = a_0^2 \geqslant 0,$$

which leads to a monokinetic solution $\varrho(t,x)\delta(\xi - u(t,x))$ at least for some time if ϱ_0, u_0 are smooth, [40]. Indeed, we can initialize (25) as follows:

$$X(t=0,\alpha) = X_0(\alpha), \quad U(t=0,\alpha) = u_0(X_0(\alpha)), \tag{26}$$

with X_0 the *reciprocal mapping* of ϱ_0 (i.e., the pseudo-inverse of the antiderivative of ϱ_0) in the sense of [30]. That is to say, we consider $r_0(x) = \int_{-\infty}^{x} \varrho_0(s)\cdot \mathrm{d}s$, an increasing function. There obviously holds $\lim_{x\to+\infty} r_0(x) = \|a_0(t=0,.)\|^2_{L^2(\mathbb{R})} = R$; usually $R = 1$ because of the probabilistic interpretation of the kinetic distribution. The reciprocal mapping X_0 is defined as a pseudo-inverse of r_0, i.e.,

$$\begin{aligned}&X_0 : [0,1] \to \mathbb{R}\\ &\alpha \mapsto X_0(\alpha) := \inf\ \sup\{y \in \mathbb{R} \text{ such that } r_0(y) = \alpha\}.\end{aligned} \tag{27}$$

Now, by definition (27), X_0 is a solution at time $t = 0$ of the *Jacobian equation*:

$$\varrho(t,X(t,\alpha))\left|\frac{\partial X}{\partial \alpha}(t,\alpha)\right| = 1. \tag{28}$$

Pushing further, one observes from (19) that $r(t, x)$, any antiderivative of μ, solves the transport equation $\partial_t r + E'(u)\partial_x r = 0$; hence $\alpha = r(t, X(t, \alpha)) = r_0(\alpha)$ holds before breakup. Moreover, assuming the solution of (25) and (26) being given (by a suitable extension of the recent theorems in [1,12,50]), let us consider any function $\sigma(t, x)$ satisfying (28) with $\sigma(t = 0, x) = \varrho_0(x)$. This means that for any continuous test-function $\phi \in C^0(\mathbb{R})$,

$$\int_{\mathbb{R}} \phi(X(t,\alpha))\cdot \mathrm{d}\alpha = \int_{\mathbb{R}} \phi(x)\sigma(t,x)\cdot \mathrm{d}x.$$

Then, differentiating on both sides with respect to time and using (25) leads to:

$$\int_{\mathbb{R}} \phi(x)\partial_t\sigma(t,x) = \int_{\mathbb{R}} \partial_x\phi(X(t,\alpha))E_n'(U(t,\alpha))\cdot \mathrm{d}\alpha = \int_{\mathbb{R}} \partial_x\phi(x)E_n'(u)(t,x)\cdot\sigma(t,x)\cdot \mathrm{d}x,$$

which is but a weak formulation of the continuity equation $\partial_t\sigma + \partial_x(\sigma E_n'(u)) = 0$ holding for $t \mapsto \sigma(t,.)$ smooth enough. Hence by a uniqueness result,[4] we have $\sigma(t,.) = \varrho(t,.)$ since intial data coincide.

A consequence is that for any $\phi \in C^0(\mathbb{R}^2)$ and X, U solution of (25) and (26), there holds:

$$\int_{\mathbb{R}} \delta(x - X(t,\alpha))\delta(\xi - U(t,\alpha))\phi(x,\xi)\cdot \mathrm{d}x\cdot \mathrm{d}\xi = \int_{\mathbb{R}} \phi(X,U)(t,\alpha)\cdot \mathrm{d}\alpha = \int_{\mathbb{R}} \phi(x,u(t,x))\varrho(t,x)\cdot \mathrm{d}x,$$

with $u(t,.)$ implicitly defined by $u(t, X(t,\alpha)) = U(t,\alpha)$ as long as $\alpha \mapsto X(t,\alpha)$ remains a diffeomorphism (an admissible change of variables!). This precisely means that the density built out of (25) and (26) reads $f(t,x,\xi) = \varrho(t,x)\delta(\xi - u(t,x))$ on this time interval.

3.3. Updating the intensities within a time-marching scheme

We have presented in the former section a Lagrangian framework to solve the Vlasov–Poisson Eq. (22). Following [36], the WKB strategy can be seen as a mean to manufacture a quantum wave function starting from the knowledge of the classical motion in phase space. The theory of "K-branch solutions" [16,24,46] is well-suited[5] to compute efficiently multivalued velocities $\vec{u} = \partial_x\varphi$ (or crystal momentum); it is moreover easier to handle when compared to the processing of the full moment systems emanating from a Wigner analysis, see [47,33,28,27,25]. Indeed, as the treatment of the corresponding (possibly multivalued) intensities μ is decoupled, moment systems become less singular hence less demanding at a computational level. In return, original algorithms have to be devised in order to update $\vec{\mu}$ at each time-step: in [28,25], some sort of "backwards ray-tracing" has been introduced (because the bicharacteristics are straight lines for homogeneous problems) whereas the conservation of the Hamiltonian along trajectories in phase space has been used in [26].

Both techniques fail when considering the Poisson coupling here; however, an algorithm consistent with the analysis of Section 3.1 can be easily deduced. Indeed, the right-hand side of the second equation in (25) corresponds to the field created by all the electrons located on the left of the one at $X(t,\alpha)$; this is what is needed in order to set up a semi-lagrangian scheme.

From now on, Δx and Δt will stand for the usual parameters of a cartesian grid in the t, x-plane and we assume the reader familiar with the numerical schemes of [28,26] which generate $\vec{u}_j^n = (u_{k=1,\dots,K})_j^n$, an approximation of $\vec{u}(t^n = n\Delta t, x_j = j\Delta x) \in \mathbb{R}^K$ for $j,n \in \mathbb{Z}\times\mathbb{N}$. Then let us consider an auxiliary quantity $F_k(t,x)$ at each time-step; at time $t = 0$, it is defined as follows:

$$F_k(t=0,x_j) = \int^{x_j} \mu_k(t=0,s)\cdot \mathrm{d}s = \int^{x_j} |a_0|^2(t=0,s)\cdot \mathrm{d}s, \quad k = 1,\dots,K.$$

Once again, this quantity is defined up to a constant coming from the Poisson equation. Then, as an antiderivative of μ_k, each F_k solves a transport equation $\partial_t + u_k\partial_x = 0$ (see Section 3.2), so from (18), (25) and [26] Section 3.1, we update it at every time-step like

$$F_k(t^{n+1}, x_j + E'(u_k(t^n,x_j))\Delta t) = F_k(t^n,x_j), \quad k = 1,\dots,K,$$

for some energy band $\kappa \mapsto E(\kappa)$ corresponding to the initial data (18). It is easy to interpolate the values $F_k(t^{n+1},.)$ on the original Eulerian grid $x_j = j\Delta x$ for instance by means of quadratic splines just solving a 3×3 Vandermonde system in every computational cell (see [10] for some mathematical properties of interpolation operators in a related context). Intensities $\mu_k(t^{n+1}, x_j) := \partial_x F_k(t^{n+1}, x_j)$ can be recovered by means of e.g., centered differences, as in [30].

[4] A simple energy estimate gives $\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}} \frac{\sigma^2}{2}\cdot \mathrm{d}x = -\int_{\mathbb{R}} \sigma(\partial_x\sigma)E_n'(u)\cdot \mathrm{d}x = \int_{\mathbb{R}} \frac{\sigma^2}{2}\partial_x E_n'(u)\cdot \mathrm{d}x$ which makes sense for Lipschitz u's.

[5] Namely, this "interpolation between geometric and viscosity solutions" essentially leads to $K\times K$ moment systems from which $f(t,x,\xi)$ can be exactly recovered as long as K is big enough; otherwise entropy is produced through compressive Lax shocks and irreversibility appears.

Now, in order to compute an approximation of $\vec{u}(t^{n+1}, x_j)$, a value for the electric field *independent of k* can be deduced:

$$\mathbb{R} \ni F(t^{n+1}, x_j) = \sum_{k \text{ s.t. } |F_k(t^{n+1},x_j) - F_{k-1}(t^{n+1},x_j)| > \Delta x} F_k(t^{n+1}, x_j),$$

where we chosed arbitrarily Δx to be the threshold value (this can be seen as the correct answer to the issue raised in [26], Appendix A). This means that, in case several electrons with different momenta u_k show up at x_j, the total electric field is given by summing the fields F_k produced by each electron, as written in (25). At last, the velocities can be updated by, e.g., a simple extension of the "Riemann split-schemes" of [26], Section 2.3. Of course, the aforementioned algorithm can be used for simpler cases, like for instance the ones presented in [26]. At last, in case $V'_{\text{ext}} \neq 0$, one has to include the corresponding terms in the moment system's right-hand side, see again [26].

Remark 2 (*Consistency with the* δ-closure [34]). It isn't easy at this level to state whether or not the approximate solutions (18) built out of the aforementioned algorithm are consistent with the ones obtained in [34]. First, in case K is chosen too low, they will surely be different as they already are in the linear case, as seen in [27]. Now, even if K is big enough, one should need a genuine comparison with Schrödinger computations since there is no uniqueness result for the Vlasov–Poisson equation with measure-data [50].

4. Numerical experiments

We want now to check numerically the outcome of our WKB approach by a systematic comparison with the quadratic observables coming out of a Fourier scheme [3] for the Schrödinger–Poisson equation (10) as done in [28,26] for the linear case. We shall use the same parameter, namely $\delta t = 0.01$.[6] Following [17], we tried to check on the right column a weak convergence as $\varepsilon \to 0$ by looking at the antiderivative of the difference of the position densities (the first quadratic observable); thus we shall study the function

$$x \mapsto \int_0^x (\varrho^{\varepsilon}_{\text{WKB}}(T,s) - |\psi^{\varepsilon}(T,s)|^2) \cdot \mathrm{d}s, \tag{29}$$

which can be expected to flatten as ε is decreased. $\varrho^{\varepsilon}_{\text{WKB}}$ stands for the position density obtained from the WKB ansatz (18) as done in [28,26]. Lemma 2.1 in [17] ensures that the L^1 norm of (29) going to zero is equivalent to the weak convergence of ρ^{ε}_{WKB}. It appeared *absolutely* necessary to filter numerically the input or the outcome of the Fourier schemes; here we used a standard convolution receipe involving a Gaussian kernel $\exp(-a\xi^2)$, $a \in \mathbb{R}^+$. Different values of a have been used, from 0.01 to 0.1. More precisely, to initialize the Fourier time-split schemes, we shall always use

$$\frac{1}{\sqrt{2\pi}\sqrt{\pi a}} \int_{\mathbb{R}} \psi^{\varepsilon}_n(0,s) \exp(-(x-s)^2/4a) \cdot \mathrm{d}s \Longleftrightarrow \hat{\psi}^{\varepsilon}_n(0,\xi) \exp(-a\xi^2),$$

instead of (18); of course, letting $a \to 0$, one recovers the correct initial signal.

[6] The notation Δt refers to the time-step used to compute the solution of hyperbolic moment systems. δt stands for the one used in the time-splitting Fourier schemes.

4.1. Free self-consistent electron cloud

This first test-case corresponds to (10) with constant ionic and exterior potentials; of course this leads to a trivial Bloch decomposition with a unique energy band $E(\kappa) = \frac{\kappa^2}{2}$, an infinite Brillouin zone and constant modulations involved. The WKB system (19) is just made of the classical Eikonal/continuity equations (as in [24,25]) coupled by the Poisson potential. We selected the following initial data, inspired by [27,29]:

$$u_0(x) = \sin(x)|\sin(x)|, \quad \mu_0(x) = \exp(-(x-\pi)^2)/2\pi, \tag{30}$$

which leads to a 5-branch solution after some time. The inversion routines of [29] have been used to generate the results of Fig. 1 ($T = 0.5$), Figs. 2 and 3 ($T = 2.5$), pre- and post-breakup, respectively. 512 points of discretization have been used for both methods; the CFL number has been chosen to be 0.95. Beyond caustic onset, one observes the appearance of the double cusp on Fig. 2; there is a quite good agreement between the WKB approximation and the direct Schrödinger computation in both logarithmic and normal scales away from caustics. One can observe the nice convergence in log-scale as ε is decreased on Figs. 1 and 3; interestingly, the two curves look similar despite bigger errors in the 5-valued context. Notingly, the 5-valued region $x \in [2.5,3.5]$ seems to produce the right values for the position density. Finally, it seems that the error terms coming from multivaluations

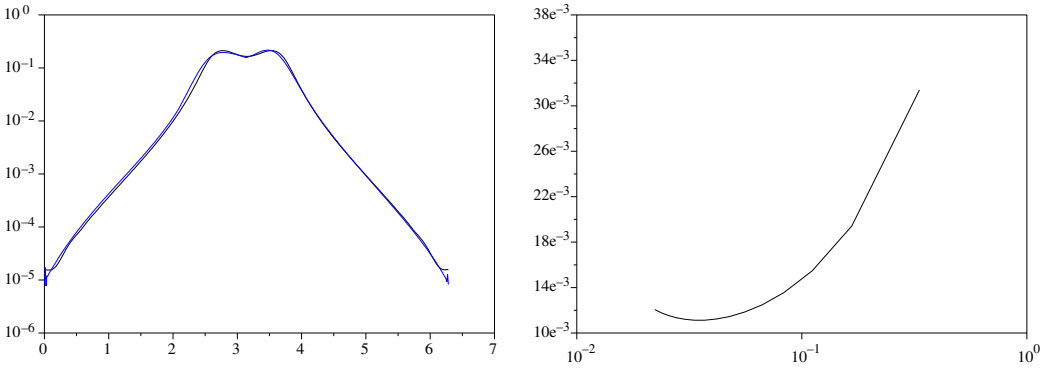

Fig. 1. Comparison of position densities in $T = 0.5$ with $\varepsilon = 1/25$ (left) and decay of (29) as $\varepsilon \to 0$ (right).

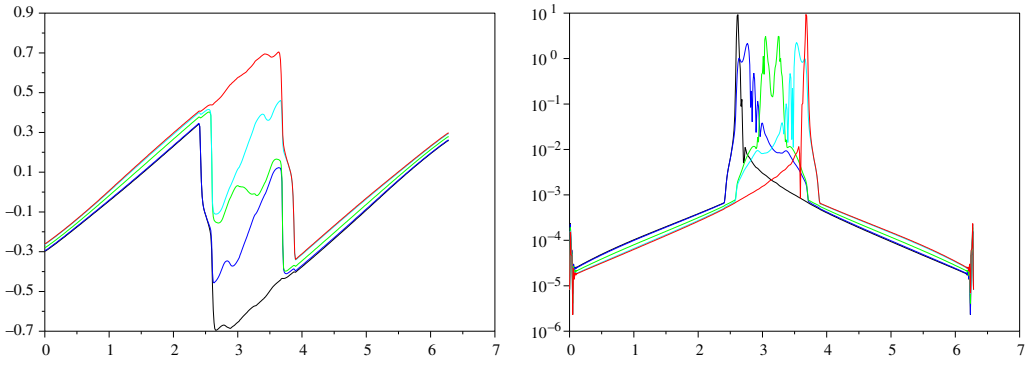

Fig. 2. 5-branch velocity (left) and corresponding intensities (right) at time $T = 2.5$.

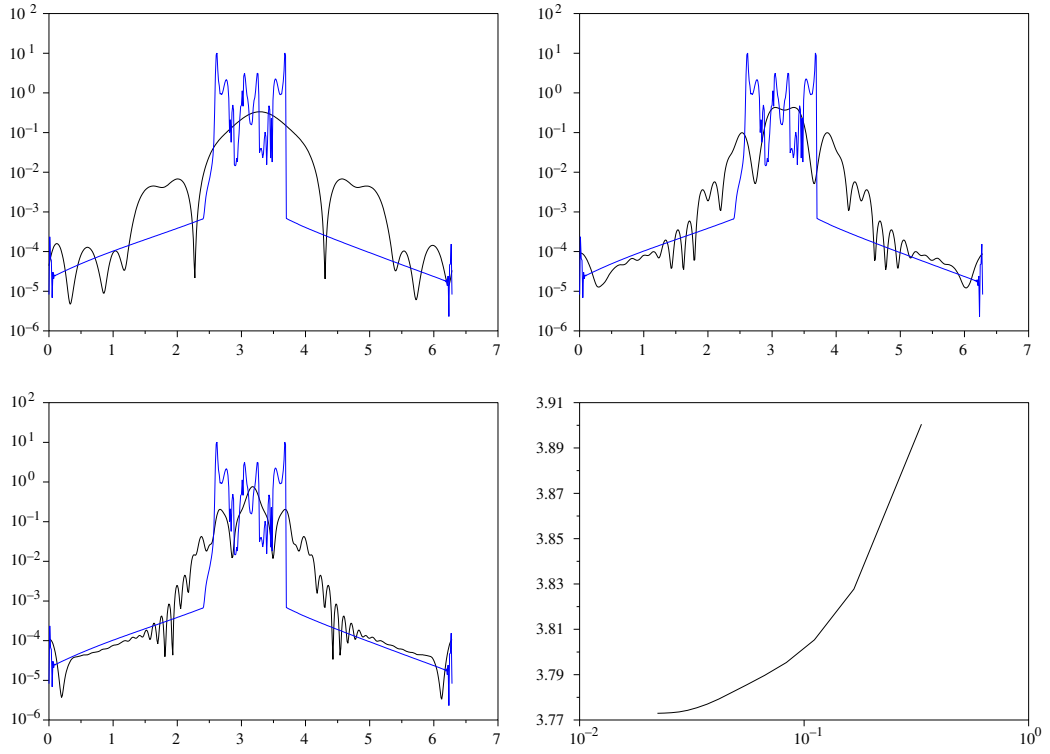

Fig. 3. Comparison of position densities in $T = 2.5$ with $\varepsilon = 1/10,1/25,1/40$ and decay of (29) as $\varepsilon \to 0$ (left to right, top to bottom).

are indeed of little influence when carrying out practical computations: this (partially) answers the question raised in Remark 1.

4.2. Self-consistent electron cloud within Mathieu's potential

This test-case corresponds to (10) with $V_{\text{ion}}(x) = \cos(x)$ and $V'_{\text{ext}} \equiv 0$. The main novelty with respect to the former one lies in the handling of the Bloch decomposition and the energy bands when computing the moment systems which govern the evolution of the K-branch solutions; this has been done according to the routines proposed in [28,26]. We selected an initial datum leading only to a 3-branch solution,

$$u_0(x) = 0.3\sin(x), \quad \mu_0(x) = 0.3\exp(-(x-\pi)^2)/\pi. \tag{31}$$

Since the Poisson term is repulsive, a strong initial position density prevents numerous multivaluations to develop in the solution. The 3-branch solutions are displayed on Fig. 4 where the dispersive effect of the repulsive Poisson term is clearly seeable. We compared with a direct Schrödinger computation at time $T = 2$, see Fig. 5. The agreement looks satisfying away from caustics; even the central spike is produced by both schemes. A decay of the L^1 norm of (29) in $T = 2$ (and even a harsh strong L^1 convergence) has also been observed,[7] see Fig. 6. The error coming from the spurious blowup on the caustics seems to decrease and the results in the multivalued region contribute at most up to 10% of the overall (as seen on

[7] Compare especially with Figs. 11 and 12 in [26].

the antiderivatives of the position densities' difference, right of Fig. 6. We believe that the slight increase of the L^1 norm of (29) as $\varepsilon \simeq 1/40$ comes from a shortage of Fourier modes; 512 points of discretization have been used here.

It is interesting to notice that one main difference with Section 4.1 is the number of multivaluations; hence part of the error reported on Fig. 3 with respect to Fig. 6 comes from the algorithm used to invert Markov's moment problem as proposed in [29]. Also the simulation of a bigger hyperbolic moment system is likely to produce slightly higher truncation errors.

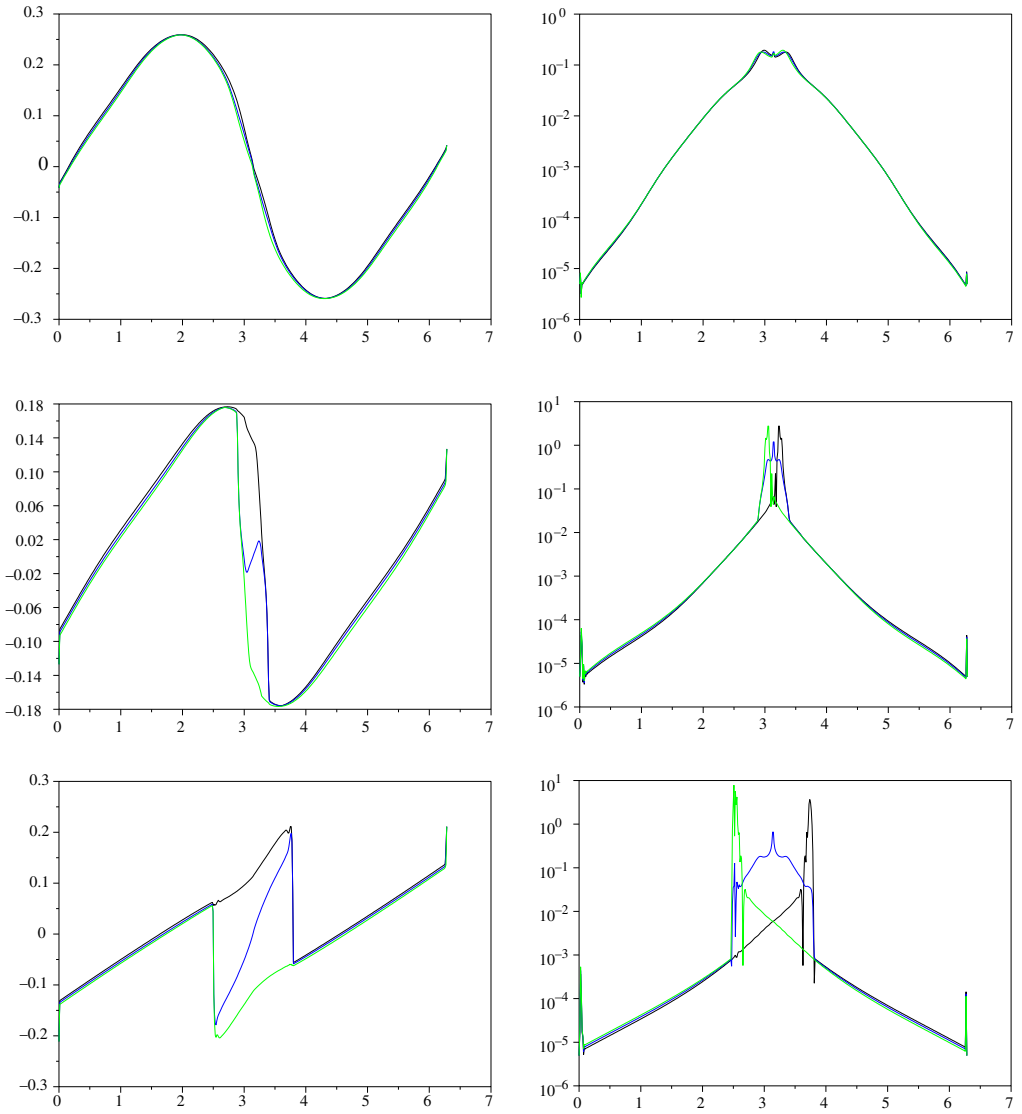

Fig. 4. 3-branch velocities (left) and corresponding intensities for Mathieu's potential at times $T = 0.5, 1.5, 2, 2.5, 3.5$ (top to bottom).

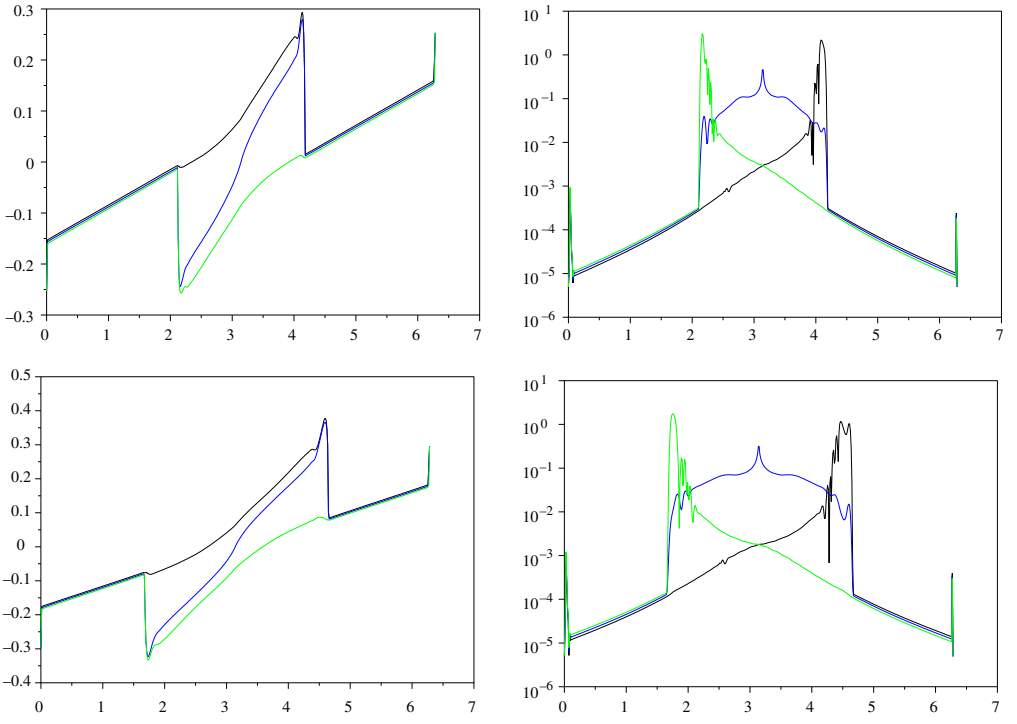

Fig. 4 (*continued*)

4.3. A smoothered model for screening

The situation described now is still given by $V_{\mathrm{ion}}(x) = \cos(x)$ supplemented by an exterior Coulomb term $V_{\mathrm{ext}}(x) = \frac{-1}{|x-x_0|}$; i.e., a potential induced by an impurity inside the periodic lattice. It has already been studied in [26] in a linear context, that is to say, without considering any self-interaction among the electrons. Roughly speaking, V_{ext} creates a potential well around x_0, but the repulsive Poisson term has the opposite effect and both mechanisms should balance after some transient regime. However, it hasn't been possible to work with the normal Coulomb term because it is too singular; hence we turned back to a smoother potential,

$$V_{\mathrm{ext}}(x) = -\cos(0.5(\pi - x))^2.$$

The initial data are rather simple:

$$u_0 \equiv 0, \quad \mu_0(x) = \exp(-(x-\pi)^2)/2\pi.$$

Results at time $T = 2$ are shown in Fig. 7. The validation is done by means of a comparison with a direct Schrödinger computation with 1024 Fourier modes in Fig. 8. It's been more difficult to obtain a reliable outcome while decreasing the parameter ε thus we show a decay of the L^1 norm of (29) only for moderate values, see Fig. 9. We notice that for $\varepsilon \in [1/25,1/5]$, the weak consistency is quite satisfying.

5. Conclusion and outlook

An extension of the Homogenization/WKB techniques to the weakly nonlinear Schrödinger–Poisson equation has been introduced, in the spirit of [7,50]. It somehow "closes a loop" initiated in the joint

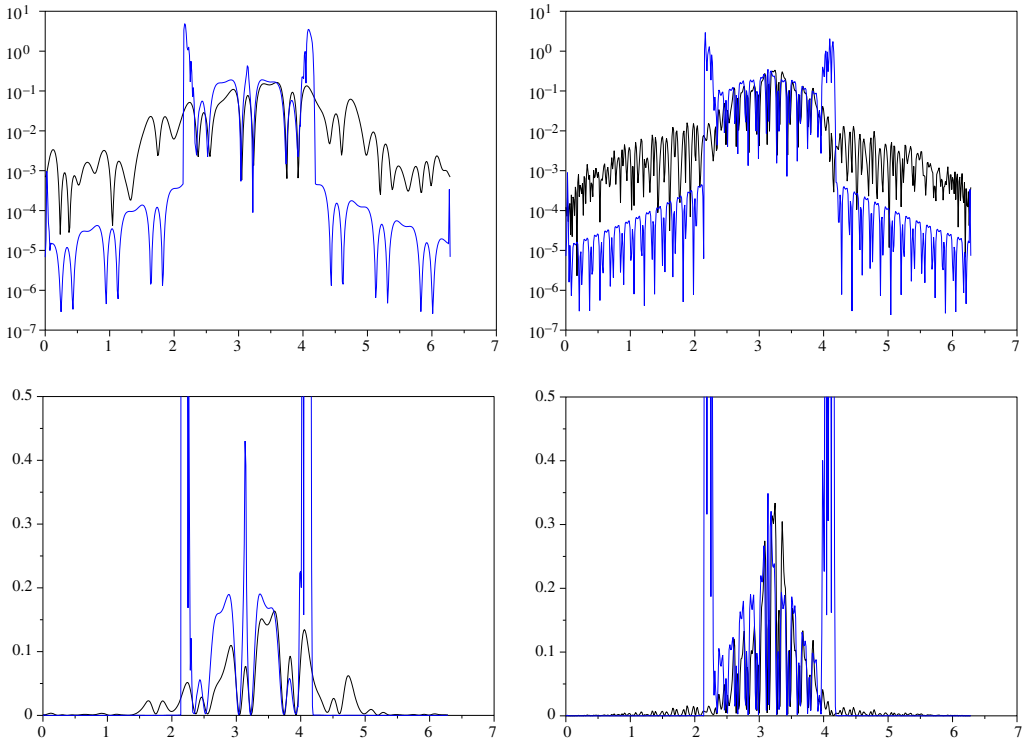

Fig. 5. Comparison of position densities in $T = 2.5$ with $\varepsilon = 1/10$ (left) and $\varepsilon = 1/40$ (right) in logarithmic (top) and normal (bottom) scales.

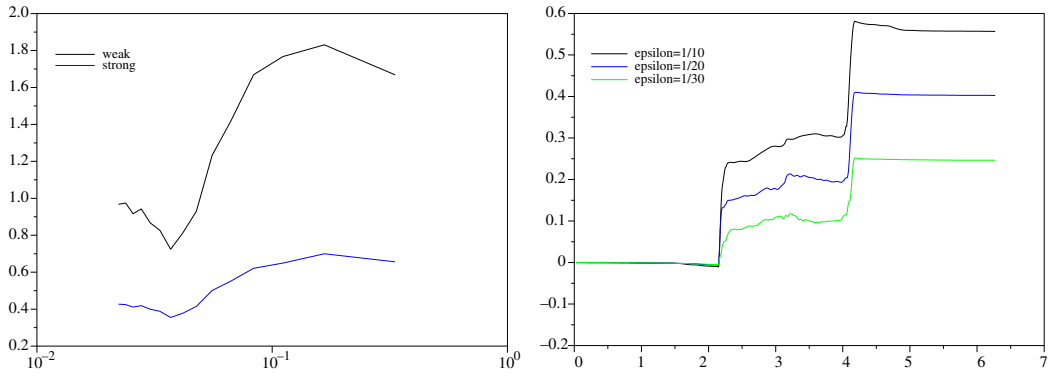

Fig. 6. Decay of the L^1 norm of (29) and $\|\varrho^{\varepsilon}_{\mathrm{WKB}}(T,.) - |\psi^{\varepsilon}(T,.)|^2\|_{L^1}$ (left); several glimpses on (29) in $T = 2.5$ as $\varepsilon \to 0$.

work [28] and the earlier ones [24,46]. The validation of our numerical algorithms has been entirely done by systematic comparisons of quadratic observables with the ones obtained from direct computations on Schrödinger–Poisson models with time-splitting Fourier schemes. A clean convergence of the position densities has been observed for problems of increasing difficulty. This confirms the results

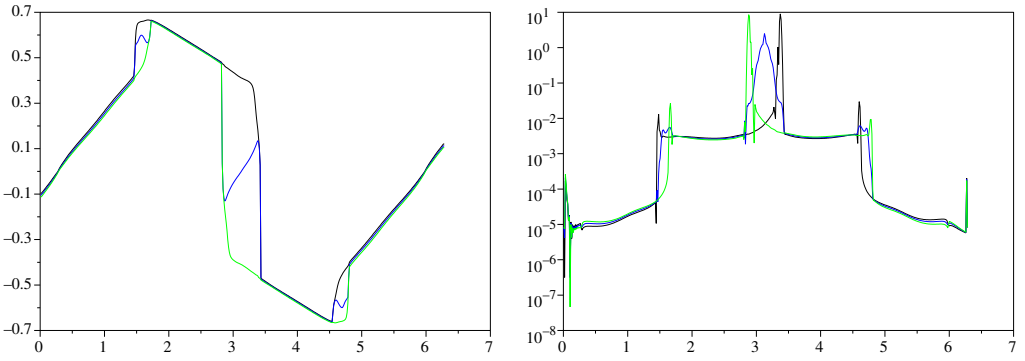

Fig. 7. 3-branch velocity (left) and corresponding intensities (right) at time $T = 2$.

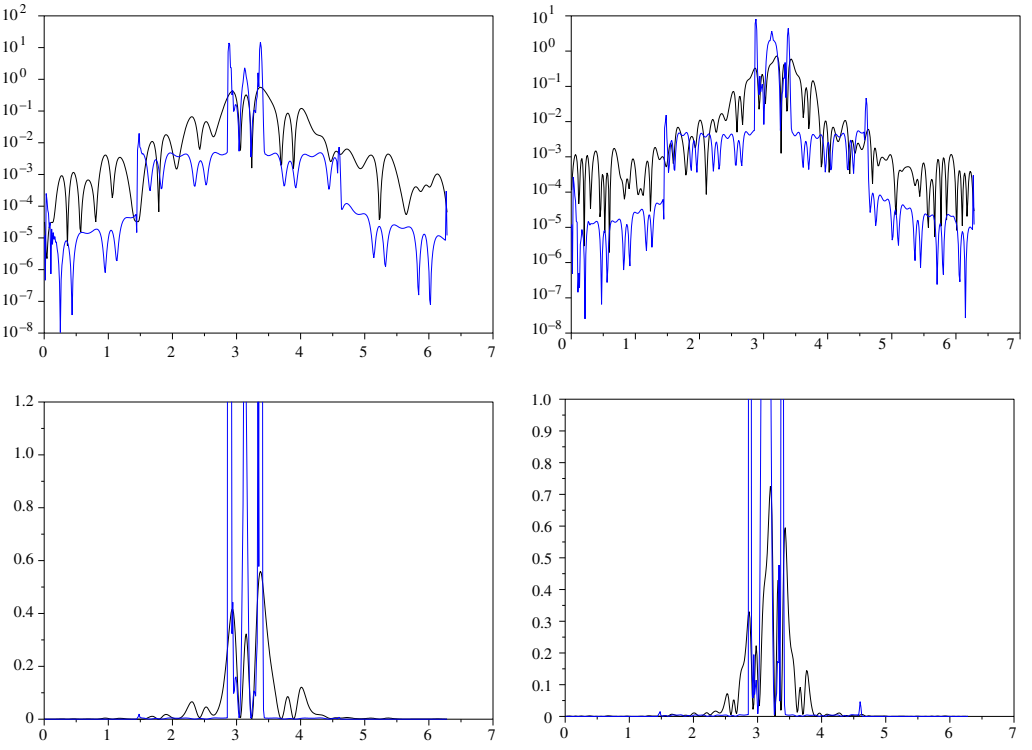

Fig. 8. Comparison of position densities in $T = 2$ with $\varepsilon = 1/9$ (left) and $\varepsilon = 1/18$ (right) in logarithmic (top) and normal (bottom) scales.

from [25] concerning the validity of these 1D WKB techniques with K-branch solutions, [16,24,29,46], even for weakly nonlinear problems of the type (1). Indeed one could be tempted to go down this track and study the semi-classical limit of the so-called $X\alpha$ equation heuristically derived in [43] which reads:

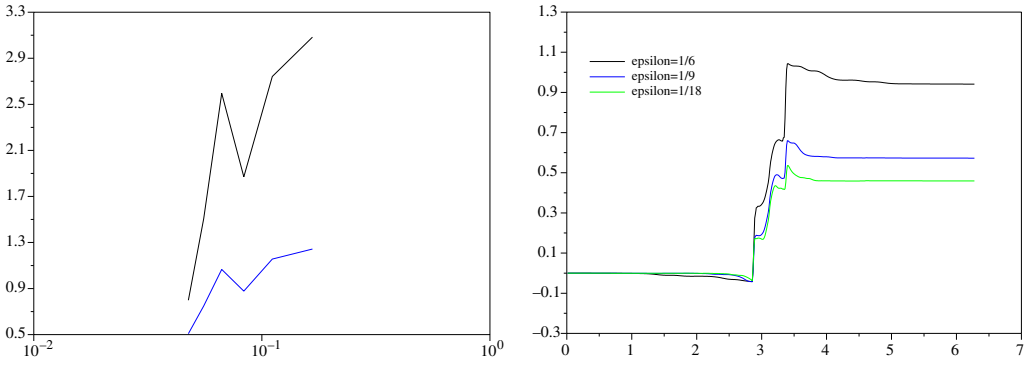

Fig. 9. Decay of the L^1 norm of (29) and $\|\varrho^{\varepsilon}_{\mathrm{WKB}}(T,.) - |\psi^{\varepsilon}(T,.)|^2\|_{L^1}$ (left); several glimpses on (29) in $T = 2$ as $\varepsilon \to 0$.

$$\mathrm{i}\hbar\partial_t\psi + \frac{\hbar^2}{2m}\partial_{xx}\psi = e(V_{\mathrm{ion}}(x) + V_{\mathrm{ext}}(x) + V_{\mathrm{P}}(t,x) - \alpha|\psi|^{\frac{2}{3}})\psi, \quad -\epsilon_0\partial_{xx}V_{\mathrm{P}} = e|\psi|^2. \tag{32}$$

The strong focusing nonlinearity emanating from Pauli's exclusion principle forbids to apply any known technique to obtain rigorously the semiclassical behaviour of ψ, see [19]. However, the local exchange term $-\alpha\rho = \alpha(\frac{\epsilon_0}{e}\partial_{xx}V_{\mathrm{P}})$ might be treated as a small perturbation (for α below a critical threshold [4]) inside the present approach. At best, this equation is likely to describe ballistic transport of electron ensembles inside solid-state materials. These basic concepts don't address the issue of collisions (phonons, impurities, see [2]); they are incorporated by linking the ballistic quantum transport picture to a classical Boltzmann-type equation and by assuming that quantum effects and collisions aren't relevant in the same computational subdomains, see [9].

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