ANALYSIS OF A SEMI-DISCRETE VERSION OF THE WIGNER EQUATION

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Abstract: We introduce a semi-discretized version of the Wigner equation, discretization concerning the velocity variable. We show that the correponding discrete velocity problem is well-posed and permits to approach the solution of the continuous problem when the mesh size of the discretization vanishes. The approximation presents spectral accuracy since the rate of convergence corresponds to the (Sobolev) regularity of the continuous solution. We also discuss the behaviour of the solution with respect to the Planck constant.

Key words: Wigner equation, Discrete velocity models, Semi-classical limit.

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1 Introduction

We are concerned with the following Wigner (or "quantum Liouville") equation

$$\partial_t f + \xi \cdot \nabla_x f = \Theta(V)(f) \qquad \text{in } \mathbb{R}^+_t \times \mathbb{R}^N_x \times \mathbb{R}^N_\xi, \tag{1}$$

where the right hand side is defined by the pseudo-differential operator

$$\Theta(V)(f) = i\mathcal{F}^{-1}_{y\to\xi}\big((V(x+y/2) - V(x-y/2))\widehat{f}(t,x,y)\big). \tag{2}$$

Throughout the paper one denotes indifferently by $\mathcal{F}(f)$ or by $\widehat{f}$ the Fourier transform given, under suitable integrability condition on f, by

$$\widehat{f}(y) = \int_{\mathbb{R}^N} e^{-iy\cdot\xi} f(\xi)\, d\xi,$$

[1]Part of this work has been performed during a stay at the Erwin Schrödinger Institute in Vienna; friendly hospitality and support by the Austrian START project "Nonlinear Schrödinger and quantum Boltzmann equations" are kindly acknowledged.

and $\mathcal{F}^{-1}(f)(\xi) = \int e^{+iy\cdot\xi} f(y)\, dy/(2\pi)^N$.

This equation is intended to model the quantum transport of electrons in a semiconductor device. The unknown $f(t,x,\xi)$ is real valued, but, contrary to what happens usually in kinetic theory, it is not naturally non negative. Usually, the electric potential V is obtained in a self-consistent way through the Poisson equation $\Delta V(t,x) = \int f\, d\xi - D(x)$, D being a given doping profile. This relation describes the Coulombian interactions between the electrons. Note that this definition is not obvious at all since the natural framework for f is the space $L^2(\mathbb{R}^N \times \mathbb{R}^N)$ so that it is not clear how the integral of f can make sense. However, here and below, we restrict ourselves to a linear situation where the potential V is given; it lies at least in $L^\infty(\mathbb{R}^N)$. Consequently, the operator $\Theta(V)$ is bounded in $L^2(\mathbb{R}^N)$ (see Lemma 2).

The equation (1) may be seen as the quantum equivalent of the classical Vlasov equation

$$\partial_t f + \xi \cdot \nabla_x f - \nabla_x V \cdot \nabla_\xi f = 0,$$

where one considers that electrons are moving along the trajectories of the Hamiltonian $\xi^2/2 + V$. Actually, the integro-differential equation (1) can be obtained by considering the Wigner transform, introduced in [14], of the solution of the Schrödinger equation with potential V. On the other hand, the Vlasov equation can be recovered as the Planck constant goes to 0 when dealing with suitabily rescaled Wigner transform. The mathematical analysis of these questions has been performed by P.L. Lions-Th. Paul [10]. We also refer for further details and results on the model to the works of P. Markowich [5], P. Markowich-C. Ringhofer [8], P. Degond-P. Markowich [3] and the classical treatise of P. Markowich-C. Ringhofer-C. Schmeiser [9]. We also quote for an extensive study and application of Wigner transform the recent paper of P. Gérard-P. Markowich-N. Mauser-F. Poupaud [4].

In this work, we wish to introduce a semi-discrete version of the Wigner equation (1) and to discuss some properties of the approximation obtained in this way. Discretization here is performed with respect to the ξ variable and we search for a discrete model that looks like (1)

$$\partial_t w_n + \xi_n \cdot \nabla_x w_n = \big(\Theta_d(V)(w)\big)_n \qquad \text{in } \mathbb{R}_t^+ \times \mathbb{R}_x^N \times \mathcal{Z}, \tag{3}$$

where $\mathcal{Z}$ is some subset of $\mathbb{Z}^N$, possibly $\mathbb{Z}^N$ itself and ξ_n belongs to a discrete set of velocities, parametrized by $n \in \mathcal{Z}$. Therefore, our aim is two-fold:

1) on one hand, the problem (3) should be well-posed, see Theorem 1;

2) on the other hand, one expects that (3) "approaches" (1) in the sense that one may construct from the w_n's a function $f^h(t, x, \xi)$ which converges to f, solution of (1) as the parameter h, related to some "mesh size", goes to 0, see Theorem 2.

This kind of question has been addressed for instance by C. Ringhofer, with a slightly different approach, in [12], [13] and in A. Arnold-C. Ringhofer [2]; more generally, we refer to the recent and complete review on computational methods for semiconductors models [11]. We also mention the work of A. Arnold-H. Lange-P. Zweifel in [1] in a monodimensional and stationary framework, with a discussion of relevant inflow boundary conditions. Here, our approach is rather close to the analysis of finite-different schemes by P.Markowich-F. Poupaud [7]. Notice also the use of Wigner transform techniques to analyze numerical schemes by P. Markowich-P. Pietra-C. Pohl [6]. The paper is organized as follows. The next section will introduce the main ideas to achieve the program: it contains basic preliminaries and notations. Section 3 is devoted to the discrete problem: having defined the discrete operator Θ_d, we analyze well-posedness of the corresponding problem (3). Roughly speaking, we use the (formal) interpretation of Θ as a convolution to define the operator Θ_d as a discrete convolution. Then, in Section 4, we define the approximation f^h from the discrete solution and show a convergence result to the solution of (1). Our method has infinite order: the rate of convergence is given by the degree of regularity on the Sobolev scale with respect to the ξ variable of the solution of the continuous problem. Eventually, Section 5 is concerned with semi-classical limit: one investigates the behaviour of the solutions as the (scaled) Planck constant goes to 0 and we show convergence to the solution of the Vlasov equation.

2 Preliminaries

Roughly speaking, the idea consists in neglecting the large values of the dual variable, which is denoted $y \in \mathbb{R}^N$, of ξ: we restrict the band length. Then, our construction relies on the following simple observation. Let $g(\xi)$ be a smooth function, in the sense that its Fourier transform has a compact support $\text{supp}(\widehat{g}) \subset B(0, R)$. Let $Y = [-L/2, +L/2]^N$ be a box in $\mathbb{R}^N$ with length $L/2$ larger than R. We denote by $L^2_\#$ the set of square integrable functions on Y, which are $Y-$periodically extended on $\mathbb{R}^N$. We associate to such a function g a function $G \in L^2_\#$ as follows

$$\begin{cases} Y = [-L/2, +L/2]^N, \qquad 0 < R < L/2, \\ G(y) = \widehat{g}(y) \quad \text{on } B(0, R), \quad G(y) = 0 \quad \text{on } Y \backslash B(0, R), \\ y \longmapsto G(y) \quad \text{is } Y-\text{periodic}. \end{cases} \tag{4}$$

A simple computation shows that the Fourier coefficients of G are given by discrete equidistributed values of g, namely one has

$$\begin{aligned} \widehat{G}(n) &= L^{-N}\int_Y e^{i2\pi y\cdot n/L}G(y)\,dy \\ &= L^{-N}\int_{\mathbb{R}^N} e^{i2\pi y\cdot n/L}\widehat{g}(y)\,dy = (2\pi/L)^N g(2\pi n/L) \end{aligned}$$

by the inversion formula. Therefore, we naturally set $g_M(\xi) = \mathcal{F}^{-1}_{y\to\xi}(\widehat{g_M})(\xi)$ with $\widehat{g_M}(y) = \sum_{|n|\leq M}\widehat{G}(n)e^{-i2\pi n\cdot y/L}\chi_{|y|\leq R}(y)$. Here and below $|y|$ and $B(0,R)$ refer to the infinite norm on $\mathbb{R}^N$ and the corresponding ball; while, for a multi-integer $n\in\mathbb{Z}^N$, $|n|$ stands for the length $|n| = |n_1| + ... + |n_N|$. This actually means that

$$\begin{aligned} g_M(\xi) &= \sum_{|n|\leq M}\int_{\mathbb{R}^N} e^{iy\cdot\xi}e^{i2\pi n\cdot y/L}\widehat{G}(n)\chi_{|y|\leq R}(y)\,dy/(2\pi)^N \\ &= \sum_{|n|\leq M}(2\pi/L)^N\;g(2\pi n/L)\int_{B(0,R)}\exp(iy\cdot(\xi-2\pi n/L))\,dy/(2\pi)^N \\ &= \sum_{|n|\leq M}\left(L^{-N}\;g(2\pi n/L)\prod_{j=1}^{N}\frac{2\sin(R(\xi_j-2\pi n_j/L))}{\xi_j-2\pi n_j/L}\right). \end{aligned}$$

Since, by definition of the Fourier series,

$$\sum_{|n|\leq M}\widehat{G}(n)e^{-i2\pi n\cdot y/L}\longrightarrow_{M\to\infty} G \qquad \text{in } L^2_\#,$$

it follows that g_M tends to g in $L^2(\mathbb{R}^N)$ as M goes to ∞. Indeed, we have

$$\begin{aligned} \|g-g_M\|^2_{L^2(\mathbb{R}^N)} &= (2\pi)^{-N}\|\widehat{g}-\widehat{g_M}\|^2_{L^2(\mathbb{R}^N)} \\ &= (2\pi)^{-N}\int_{B(0,R)}\left|\widehat{g}(y)-\sum_{|n|\leq M}\widehat{G}(n)e^{-i2\pi n\cdot y/L}\right|^2 dy \\ &\leq (2\pi)^{-N}\int_Y\left|\widehat{g}(y)-\sum_{|n|\leq M}\widehat{G}(n)e^{-i2\pi n\cdot y/L}\right|^2 dy \\ &\leq (L/(2\pi))^N\left\|G-\sum_{|n|\leq M}\widehat{G}(n)e^{-i2\pi n\cdot y/L}\right\|^2_{L^2_\#(Y)} \end{aligned}$$

Let us summarize these simple facts in the following claim (which is known as the Shannon sampling theorem in signal processing).

Lemma 1 *Let $g(\xi)$ be a smooth function whose Fourier transform has a compact support* $\mathrm{supp}(\widehat{g}) \subset B(0,R)$. *Let $Y = [-L/2, +L/2]^N$ with $L/2 > R$ and set*

$$g_M(\xi) = \sum_{|n|\leq M} \left(L^{-N} \ g(2\pi n/L) \prod_{j=1}^{N} \frac{2\sin(R(\xi_j - 2\pi n_j/L))}{\xi_j - 2\pi n_j/L} \right).$$

Then, one has $\lim_{M\to\infty} \|g - g_M\|_2 = 0$.

Remark 1 *In equation (1) the unknown f is obtained as the Wigner transform of some density matrix; in turn, the density $\rho(t,x) = \int f \, d\xi$ makes sense and remains non negative, see [10]. It is worth remarking that if g is given through a truncated Wigner transform, namely*

$$g(x,\xi) = \int_{\mathbb{R}^N} \psi(x + y/2) \ \overline{\psi(x - y/2)} \ \chi_{|y|\leq R} \, e^{iy\cdot\xi} \, dy/(2\pi)^N$$

with, say, $\psi \in L^2(\mathbb{R}^N)$ (for the sake of simplicity); then, the associated discrete density remains non negative. This means that

$$\begin{aligned} \sum_{n\in\mathbb{Z}^N} \widehat{G}(x,n) &= \sum_{n\in\mathbb{Z}^N} \widehat{G}(x,n) e^{in\cdot 0} = G(0) \\ &= \widehat{g}(x,0) = \Big(\psi(x+y/2) \ \overline{\psi(x-y/2)} \ \chi_{|y|\leq R}\Big)\Big|_{y=0} = \psi(x) \ \overline{\psi(x)} \geq 0. \end{aligned}$$

For future use, let us set up here the notations and classical formulae. For f, g in $L^2_\#$, we set

$$\begin{cases} \big(f,g\big)_{L^2_\#} = L^{-N} \displaystyle\int_Y f(y)\overline{g(y)} \, dy, \qquad \|f\|^2_{L^2_\#} = L^{-N} \displaystyle\int_Y |f(y)|^2 \, dy \\ \widehat{f}(n) = \big(f, e^{-i2\pi y\cdot n/L}\big)_{L^2_\#} = L^{-N} \displaystyle\int_Y f(y) e^{+i2\pi y\cdot n/L} \, dy. \end{cases}$$

Note that in this definition the norm on $L^2_\#$ depends on the size of the box. For (complex-valued) sequences u, v in $\ell^2 = \ell^2(\mathbb{Z}^N)$, we set

$$\big(u,v\big)_{\ell^2} = \sum_{n\in\mathbb{Z}^N} u_n \overline{v_n}.$$

Of course, one has the Parseval formula

$$\big(f,g\big)_{L^2_\#} = \sum_{n\in\mathbb{Z}^N} \widehat{f}(n)\overline{\widehat{g}(n)} = \big(\widehat{f}, \widehat{g}\big)_{\ell^2} \tag{5}$$

which holds for functions f, g in $L^2_\#$. We will also use the notation

$$(u * v)_n = \sum_{k\in\mathbb{Z}^N} u_k v_{n-k},$$

and we recall that, when u or v belongs to ℓ^1, one has

$$\sum_{n\in\mathbb{Z}^N} (u * v)_n = \sum_{n\in\mathbb{Z}^N} u_n \sum_{n\in\mathbb{Z}^N} v_n. \tag{6}$$

3 The discrete problem

3.1 The discrete operator

We recall that the Vlasov-Wigner operator (2) reads

$$\Theta(V)(f)(\xi) = i\mathcal{F}^{-1}_{y\to\xi}(D_V \widehat{f})(\xi) = i\int_{\mathbb{R}^N} e^{i\xi\cdot y} D_V(x, y)\widehat{f}(y)\, dy/(2\pi)^N,$$

where we note

$$D_V(x, y) = V(x + y/2) - V(x - y/2).$$

Then, the Parseval equality gives

$$\begin{aligned} \|\Theta(V)(f)\|_2 &= (2\pi)^{-N/2}\|\mathcal{F}\big(\Theta(V)(f)\big)\|_2 = (2\pi)^{-N/2}\|D_V\mathcal{F}(f)\|_2 \\ &\leq 2(2\pi)^{-N/2}\|V\|_\infty\|\mathcal{F}(f)\|_2 = 2\|V\|_\infty\|f\|_2. \end{aligned}$$

As mentioned in the Introduction, one deduces the following statement.

Lemma 2 *Let V belong to $L^\infty(\mathbb{R}^N)$. The operator $\Theta(V)$ is continuous on $L^2(\mathbb{R}^N)$ with norm $\|\Theta\|_{\mathcal{L}(L^2(\mathbb{R}^N))} \leq 2\|V\|_\infty$.*

Let us consider the action of this operator on the smooth function g studied in the previous section. The support property implies that

$$\Theta(V)(g)(\xi) = i\int_{B(0,R)} e^{i\xi\cdot y} D_V(x, y)\widehat{g}(y)\, dy/(2\pi)^N.$$

Since $\Theta(V)$ is continuous on $L^2(\mathbb{R}^N)$, by Lemma 1 $\Theta(V)(g_M)$ converges to $\Theta(V)(g)$ in $L^2(\mathbb{R}^N)$ as $M \to \infty$. However, we get

$$\begin{aligned}
\Theta(V)(g_M)(\xi) &= i \int_{B(0,R)} D_V(x,y)\widehat{g_M}(y)e^{i\xi\cdot y}\, dy/(2\pi)^N \\
&= i \sum_{|n|\le M} \widehat{G}(n) \int_{B(0,R)} D_V(x,y)e^{i(\xi-2\pi n/L)\cdot y}\, dy/(2\pi)^N \\
&= \sum_{|n|\le M} g(2\pi n/L)\ a(\xi - 2\pi n/L)
\end{aligned} \tag{7}$$

where

$$a(\zeta) = i\ L^{-N} \int_{B(0,R)} D_V(x,y)e^{i\zeta\cdot y}\, dy. \tag{8}$$

These formulae will be our guide to write a relevant discrete operator.

In order to construct a discrete model, we set for $n \in \mathbb{Z}^N$ and a mesh size $h > 0$,

$$\xi_n = 2\pi n h$$

and we interpret the w_n's, that will be naturally searched for in ℓ^2, as the Fourier coefficients of a function $G \in L^2_\#$ with a $h-$dependent box $Y^h = [-1/(2h), +1/(2h)]^N$

$$G(y) = \sum_{n\in\mathbb{Z}^N} w_n e^{-i2\pi h y\cdot n} \in L^2_\#(Y^h).$$

This idea is reminiscient to the deep interpretation of finite difference schemes by the pseudo-differential formalism by P. Markowich-F. Poupaud [7]. According to (7-8), we define the discrete operator by convolution

$$\begin{cases} \Big(\Theta_d(V)(w)\Big)_n = \sum_k w_k a_{n-k} = (a * w)_n, \\ a_n = i\ h^N \displaystyle\int_{\mathbb{R}^N} D_V(x,y)\chi_{|y|\le R^h}(y)\ e^{i2\pi h n\cdot y}\, dy. \end{cases} \tag{9}$$

Notice that now the truncation acts on the potential with a radius $R^h < (2h)^{-1}$, where R^h is a sequence of positive numbers which tends to ∞ as $h \to 0$: one truncates the frequencies at a level less than the inverse of twice the mesh size. Following (4), one introduces

$$\begin{cases} \mathcal{V}(y) = D_V(x,y)\chi_{|y|\le R^h}(y) \text{ on } B(0,R^h), \qquad \mathcal{V}(y) = 0 \text{ on } Y^h\backslash B(0,R^h), \\ y \longmapsto \mathcal{V}(y) \quad \text{is } Y^h\text{-periodic} \end{cases} \tag{10}$$

so that $\frac{1}{i}\, a_n$ appears as the nth Fourier coefficient of the Y^h-periodic function $\mathcal{V}$. Remark also that $\mathcal{V} \in L^\infty_\#$. Therefore, we are concerned with the following discrete problem

$$\begin{cases} \partial_t w_n + \xi_n \cdot \nabla_x w_n = \Big(\Theta_d(V)(w)\Big)_n & \text{in } \mathbb{R}^+_t \times \mathbb{R}^N_x \times \mathbb{Z}^N_n, \\ w_n(t=0,x) = w^0_n(x). \end{cases} \tag{11}$$

It is not clear at all that (9) defines a bounded operator on the natural functional space ℓ^2 for the w_n's since nothing, up to additional regularity assumptions on V, ensures that a belongs to ℓ^1 (see [1] for some comments on this difficulty). However, we are able to establish this property, which is the discrete analog of Lemma 2.

Proposition 1 *The operator Θ_d is a bounded linear operator on ℓ^2 and its norm is estimated uniformly with respect to h by $\|\Theta_d\|_{\mathcal{L}(\ell^2)} \leq 2\|V\|_\infty$. Furthermore, the coefficients a_n which define the operator Θ_d are real and even; in turn, the operator is skew-symmetric.*

Proof. Let f and g be two functions in $L^2_\#$. In particular, we notice that the product fg lies in $L^1_\#$ and, consequently the Fourier coefficients $\widehat{fg}$ belong to ℓ^∞. We shall use the following relation

$$\widehat{fg}(n) = \widehat{f} * \widehat{g}(n). \tag{12}$$

Note also that if $f \in L^2_\#$ and $g \in L^\infty_\#$ one has $fg \in L^2_\#$; therefore, the corresponding coefficients $\widehat{fg}(n) = \widehat{f} * \widehat{g}(n)$ also belong to ℓ^2.

Here, the operator Θ_d is defined by

$$\Big[\Theta_d(v)w\Big](n) = a * w(n) = i\Big(\widehat{\mathcal{V}} * \widehat{G}\Big)(n) = i\widehat{\mathcal{V}G}(n)$$

by using the definitions (9) and (10), while G is the function in $L^2_\#$ having the w_n's as Fourier coefficients. Then it yields (recall that the norm $\|\cdot\|_{L^2_\#}$ depends on the size of the box Y^h)

$$\|\Theta_d(V)w\|_{\ell^2} = \|\widehat{\mathcal{V}G}\|_{\ell^2} = \|\mathcal{V}G\|_{L^2_\#} \leq \|\mathcal{V}\|_{L^\infty_\#}\|G\|_{L^2_\#} \leq 2\|V\|_{L^\infty}\|w\|_{\ell^2}$$

which proves the boundedness of Θ_d.

Let us go back to (12). Relation (5) yields

$$\big(fg,\varphi\big)_{L^2_\#} = \sum_{n\in\mathbb{Z}^N} \widehat{fg}(n)\overline{\widehat{\varphi}(n)} = \big(f,\overline{g}\varphi\big)_{L^2_\#} = \sum_{n\in\mathbb{Z}^N} \widehat{f}(n)\overline{\widehat{\overline{g}\varphi}(n)} \tag{13}$$

where φ is a regular enough test function (so that $\widehat{\varphi} \in \ell^1$ for instance). We can write, by using (6)

$$\overline{g}\varphi(y) = \sum_{n\in\mathbb{Z}^N} \widehat{\overline{g}\varphi}(n) e^{-i2\pi n\cdot y/L} = \sum_{n\in\mathbb{Z}^N} \left(\sum_{k\in\mathbb{Z}^N} \widehat{\varphi}(k)\widehat{\overline{g}}(n-k) \right) e^{-i2\pi n\cdot y/L},$$

which leads to

$$\widehat{\overline{g}\varphi}(n) = \sum_{k\in\mathbb{Z}^N} \widehat{\varphi}(k)\widehat{\overline{g}}(n-k) = \widehat{\varphi} * \widehat{\overline{g}}(n)$$

Notice that

$$\widehat{\overline{g}}(n) = L^{-N} \int_Y e^{+in\cdot z}\overline{g(z)}\, dz = \overline{L^{-N} \int_Y e^{-in\cdot z} g(z)\, dz} = \overline{\widehat{g}(-n)}.$$

Let us assume temporarily that f and g are also regular functions. We can perform the following computations from (13)

$$\begin{aligned} \left(fg, \varphi\right)_{L^2_\#} &= \sum_{n\in\mathbb{Z}^N} \widehat{f}(n) \left(\overline{\sum_{k\in\mathbb{Z}^N} \widehat{\varphi}(k)\overline{\widehat{g}(k-n)}} \right) \\ &= \sum_{n\in\mathbb{Z}^N} \widehat{f}(n) \left(\sum_{k\in\mathbb{Z}^N} \overline{\widehat{\varphi}(k)}\widehat{g}(k-n) \right) \\ &= \sum_{k\in\mathbb{Z}^N} \left(\sum_{n\in\mathbb{Z}^N} \widehat{f}(n)\widehat{g}(k-n) \right) \overline{\widehat{\varphi}(k)} \end{aligned}$$

by using Fubini's theorem (which requires the regularity of the functions). Identifying with the second term in (13), we are led to

$$\left(fg, \varphi\right)_{L^2_\#} = \sum_{k\in\mathbb{Z}^N} \left(\widehat{f} * \widehat{g}\right)(k)\overline{\widehat{\varphi}(k)} = \sum_{k\in\mathbb{Z}^N} \widehat{fg}(k)\overline{\widehat{\varphi}(k)}.$$

Since this holds for any test function φ, one actually has

$$\widehat{fg}(k) = \widehat{f} * \widehat{g}(k).$$

By a suitable regularization of f and g, but keeping φ regular, we justify this equality, that holds in ℓ^∞, for f and g in $L^2_\#$.

Finally, let us investigate the other properties of the operator Θ_d. We recall that

$$a_n(x) = i\ h^N \int_{\mathbb{R}^N} D_V(x,y) e^{i2\pi h n\cdot y} \chi_{|y|\leq R^h}\, dy.$$

Therefore, we get (with $z=-y$ and using $D_V(x,y) = -D_V(x,-y)$)

$$\begin{aligned}
\overline{a_n} &= \overline{i\ h^N \int_{\mathbb{R}^N} D_V(x,y) e^{i2\pi h n\cdot y} \chi_{|y|\leq R^h}\, dy} \\
&= -i\ h^N \int_{\mathbb{R}^N} D_V(x,y) e^{-i2\pi h n\cdot y} \chi_{|y|\leq R^h}\, dy \\
&= i\ h^N \int_{\mathbb{R}^N} D_V(x,z) e^{i2\pi h n\cdot z} \chi_{|z|\leq R^h}\, dz = a_n \\
&= -i\ h^N \int_{\mathbb{R}^N} D_V(x,y) e^{i2\pi h(-n)\cdot y} \chi_{|y|\leq R^h}\, dy = -a_{-n}
\end{aligned}$$

which proves that the coefficients a_n are real and even. In turn, we readily check that Θ_d is skew-symmetric. □

Let us conclude with some remarks. Since the discrete operator (9) is essentially obtained by truncating the potential, it will be convenient to discuss some properties of the following approximate operator

$$\Theta^h(V)(f) = \mathcal{F}^{-1}_{y\to\xi}\big(D_V\ \chi_{|y|\leq R^h}\ \widehat{f}(y)\big)$$

defined for any $f \in L^2(\mathbb{R}^N)$. The proof of the following claim is quite obvious.

Lemma 3 *The approximated operator Θ^h fulfills the following properties:*
i) if $\mathrm{supp}(\widehat{f}) \subset B(0,R)$ with $0 < R \leq R^h$, then $\Theta^h(f) = \Theta(f)$;
ii) $\Theta^h(V)(f)$ converges to $\Theta(f)$ in $L^2(\mathbb{R}^N)$ as $h \to 0$. If, furthermore, f lies in the Sobolev space $H^s(\mathbb{R}^N)$, $s > 0$, we get

$$\|\Theta^h(V)(f) - \Theta(V)(f)\|^2_{L^2(\mathbb{R}^N\times\mathbb{R}^N)} \leq \frac{4\|V\|^2_\infty}{(2\pi)^N}\ \|f\|^2_{H^s(\mathbb{R}^N)}/(1+(R^h)^2)^s.$$

As an example, it is maybe worth writing the discrete problem in a usual matrix form, when considering the mono-dimensional situation and restricting to $2M+1$ unknowns $(w_{-M},...,w_M) = W$. One gets

$$\partial_t W + \Lambda \partial_x W = AW$$

where Λ is the $(2M+1)\times(2M+1)$ diagonal matrix $\Lambda = \mathrm{diag}(\xi_{-M},...,\xi_M)$ while the coefficients of $A \in \mathcal{M}_{(2M+1)\times(2M+1)}$ are defined by

$$A_{nk} = a_{n-k}(x) = i\ h \int_{-R^h}^{+R^h} D_V(x,y) e^{i2\pi h(n-k)y}\,dy.$$

A short computation leads to

$$A_{nk} = 4h \int_{x-R^h/2}^{x+R^h/2} V(z)\sin(4\pi h(n-k)(x-z))\,dz.$$

One sees easily on this formula that A is skew-symmetric.

3.2 Analysis of the discrete problem

It is now quite easy to prove existence-uniqueness for the discrete problem (11). It is convenient here to interpret $\ell^2(\mathbb{Z}^N) = L^2(\mathbb{Z}^N, dn)$ where dn stands for the counting measure on $\mathbb{Z}^N$ and to introduce

$$L^2(\mathbb{R}^N_x \times \mathbb{Z}^N_n) = \Big\{ w : (x,n) \in \mathbb{R}^N_x \times \mathbb{Z}^N_n \longmapsto w(x,n) \in \mathbb{C}, \\ \text{such that} \int_{\mathbb{R}^N_x \times \mathbb{Z}^N_n} |w(x,n)|^2\,dx\,dn = \sum_{n\in\mathbb{Z}^N} \int_{\mathbb{R}^N_x} |w(x,n)|^2\,dx < \infty \Big\}.$$

Accordingly, in what follows, it is convenient to denote by $u(n)$ instead of u_n for the nth term of a sequence u parametrized by $n \in \mathbb{Z}^N$. When no confusion can arise we will also drop the variables t, x.

Theorem 1 *Let $w^0 \in L^2(\mathbb{R}^N_x \times \mathbb{Z}^N_n)$ and $V \in L^\infty(\mathbb{R}^N)$. The problem (11) has a unique mild solution $w \in C^0([0,T]; L^2(\mathbb{R}^N_x \times \mathbb{Z}^N_n))$. Furthermore, if the initial data w^0 is real valued (i.e. $w^0(x,n) = \overline{w^0(x,n)}$ for all $n \in \mathbb{Z}^N$ and a. a. $x \in \mathbb{R}^N$) then, the solution w remains real valued and the following relation*

$$\|w(t)\|_{L^2(\mathbb{R}^N\times\mathbb{Z}^N)} = \|w^0\|_{L^2(\mathbb{R}^N\times\mathbb{Z}^N)} \tag{14}$$

holds.

Proof. The proof is quite classical and the argument is the same as for the continuous problem in [3], [8]. Let w be a solution of (11) and let us set $w^\#(s;t,x,n) = w(t+s, x+s\xi_n, n)$. It satisfies

$$\frac{d}{ds} w^\# = \Big(\Theta_d(V)w\Big)^\#.$$

Thus, integrating leads to

$$w(t,x,n) = w^{\#}(0;t,x,n) = w^0(x - t\xi_n, n) + \int_0^t \Theta_d(V) w(\tau, x - (t-\tau)\xi_n, n)\, d\tau.$$

Let us introduce the norm

$$N(w) = \sup_{0\le t\le T} \left(e^{-\gamma t}\|w(t)\|_{L^2}\right), \qquad \gamma > K = \|\Theta_d(V)\|.$$

Then, we define an iterative scheme as follows

$$\begin{aligned} &w^{(0)}(t,x,n) = w^0(x,n),\\ &w^{(k+1)}(t,x,n) = w^0(x - t\xi_n, n) + \int_0^t \Theta_d(V) w^{(k)}(\tau, x-(t-\tau)\xi_n, n)\, d\tau. \end{aligned}$$

We readily check that

$$e^{-\gamma t}\|w^{(k+1)}(t) - w^{(k)}(t)\| \le N(w^{(k)} - w^{(k-1)})\, K/\gamma.$$

Since $K/\gamma < 1$, the scheme is contractant for the norm N, and therefore the problem has a unique solution. Since the $a(n)$'s are real, one deduces now that

$$\overline{\Theta_d(w)(n)} = \overline{\sum_{k\in\mathbb{Z}^N} a(n-k)w(k)} = \sum_{k\in\mathbb{Z}^N} a(n-k)\overline{w(k)} = \Theta_d(\overline{w})(n).$$

It follows that $\overline{w(n)}$ satisfies the same equation as $w(n)$; hence, if $w^0(n) = \overline{w^0(n)}$, one still has $w(n) = \overline{w(n)}$. In other words, w is real valued.

Finally, we are left with the task of proving the relation (14) in $L^\infty(\mathbb{R}^+, L^2(\mathbb{R}^N \times \mathbb{Z}^N,\, dx \otimes dn))$. Indeed, multiplying the equation (11) by $\overline{w_n^h}$ and integrating yield

$$\|w^h(t)\|^2_{L^2(\mathbb{R}^N\times\mathbb{Z}^N)} + \int_0^t \int \big(\Theta_d(w), w\big)_{\ell^2}(s,x)\, dx\, ds = \|w^h(0)\|^2_{L^2(\mathbb{R}^N\times\mathbb{Z}^N)}.$$

Since $\big(\Theta_d(w), w\big)_{\ell^2} \in i\mathbb{R}$, one obtains immediately (14). □

4 Approximation and convergence analysis

4.1 Construction of the approximation

In the previous section, we have obtained a sequence, parametrized by $t \in \mathbb{R}^+$ and $x \in \mathbb{R}^N$, $\big(w(t,x,n)\big)_{n\in\mathbb{Z}^N} \in \ell^2$ solution of (11). Of course, this sequence depends on the parameter h through the truncation acting on the potential and the definition of the discrete velocities $\xi_n = 2\pi nh$. We emphasize this dependence from now on by denoting the solution $w^h(t,x,n)$.

According to the strategy described in Section 2, let us introduce now for $(t,x,\xi) \in \mathbb{R}^+ \times \mathbb{R}^N \times \mathbb{R}^N$ the function

$$f^h(t,x,\xi) = \mathcal{F}^{-1}_{y\to\xi}\Big(\sum_{n\in\mathbb{Z}^N} w^h(t,x,n)\ e^{-i2\pi hy\cdot n}\ \chi_{|y|\le R^h}\Big).$$

It is maybe more explicit to write, as in Lemma 1,

$$f^h(t,x,\xi) = \sum_{n\in\mathbb{Z}^N} \left(w^h(t,x,n)\ \prod_{j=1}^{N} \frac{\sin(R^h(\xi_j - 2\pi h n_j))}{\pi(\xi_j - 2\pi h n_j)} \right).$$

Since we naturally choose $R^h \sim (2h)^{-1}$ for h small, this indicates that $f(\xi_n)$ is approximated by $(2\pi h)^{-N} w^h_n$.

Our final aim is to show that f^h approaches the solution f of (1) as the mesh size h goes to 0. Notice that here f is approximated by a formula looking like $\sum_{n\in\mathbb{Z}^N} w^h(t,x,n)S^h(\xi - \xi_n)$. In comparizon to [12], [13], instead of approaching f by periodic functions, we use an expansion on cardinal sinus functions. In [12], [13] difficulties arise since one uses a basis of functions that are not elements of the same space as the exact solution; in turn, our proof of convergence becomes very simple.

To this end, one has naturally to prepare in a suitable way the initial data $w^{h,0}$ for the discrete problem (11). It is obtained by regularizing the initial data f^0 of the continuous problem. Precisely, we set, still using the arguments of Section 2,

$$\begin{cases} f^{h,0}(x,\xi) = \mathcal{F}^{-1}_{y\to\xi}\big(\widehat{f^0}(x,y)\ \chi_{|y|\le R^h}\big), \\ G^{h,0}(x,y) = \widehat{f^0}(x,y) \quad \text{on } B(0,R^h), \qquad G^{h,0}(x,y) = 0 \quad \text{on } Y^h \backslash B(0,R^h), \\ G^{h,0}(x,y) = \quad \text{is } Y^h\text{−periodic}, \\ w^{h,0}(x,n) = \widehat{G^{h,0}(x,\cdot)}(n) = f^{h,0}(x, 2\pi nh)(2\pi h)^N, \end{cases}$$

where f^0 is real valued and belongs to $L^2(\mathbb{R}^N \times \mathbb{R}^N)$. This construction leads to the following behaviour of the discrete solution with respect to h.

Lemma 4 *One has the estimate* $\|w^{h,0}\|^2_{L^2(\mathbb{R}^N\times\mathbb{Z}^N)} \le (2\pi h)^N\ \|f^0\|^2_{L^2(\mathbb{R}^N\times\mathbb{R}^N)}$. *Consequently, one deduces that* $\|w^h(t)\|^2_{L^2(\mathbb{R}^N\times\mathbb{Z}^N)} \le (2\pi h)^N\ \|f^0\|^2_{L^2(\mathbb{R}^N\times\mathbb{R}^N)}$.

Proof. The estimate on the solution w^h is an immediate consequence of (14) combined to the estimate on the initial data. By construction, one has

$$\begin{aligned}
\|w^{h,0}\|_{\ell^2}^2 &= \|\widehat{G^{h,0}}\|_{\ell^2}^2 = \|G^{h,0}\|_{L^2_\#}^2 \\
&= h^N \int_{Y^h} |G^{h,0}(y)|^2 \, dy = h^N \int_{\mathbb{R}^N} |\widehat{f^{h,0}}(y)|^2 \, dy \\
&= h^N \int_{\mathbb{R}^N} |\widehat{f^0}(y)\chi_{|y|\le R^h}|^2 \, dy \le h^N \ (2\pi)^N \ \|f^0\|_{L^2(\mathbb{R}^N)}^2,
\end{aligned}$$

which establishes Lemma 4. □

One deduces that f^h is a bounded sequence in the natural functional space.

Corollary 1 *The sequence $\left(f^h\right)_{h>0}$ is bounded in $L^\infty(\mathbb{R}^+, L^2(\mathbb{R}^N \times \mathbb{R}^N))$. Furthermore, f^h is real valued.*

Proof. This is a consequence of Lemma 1 and Lemma 4. It is convenient to introduce the Y^h-periodic function G^h defined by the coefficients w^h_n

$$G^h(t,x,y) = \sum_{n\in\mathbb{Z}^N} w^h(t,x,n) \ e^{-i2\pi hy\cdot n} \qquad \in L^\infty(\mathbb{R}^+, L^2(\mathbb{R}^N; L^2_\#(Y^h))).$$

We have (omiting t, x variables for the sake of clarity)

$$\begin{aligned}
\|f^h\|_{L^2(\mathbb{R}^N_\xi)}^2 &= (2\pi)^{-N} \ \|\widehat{f^h}\|_{L^2(\mathbb{R}^N_y)}^2 = (2\pi)^{-N} \int_{\mathbb{R}^N} \Big| \sum_{n\in\mathbb{Z}^N} w^h(n) \ e^{-i2\pi hy\cdot n} \Big|^2 \chi_{|y|\le R^h} \, dy \\
&= (2\pi)^{-N} \int_{B(0,R^h)} \Big| \sum_{n\in\mathbb{Z}^N} w^h(n) \ e^{-i2\pi hy\cdot n} \Big|^2 \ dy \\
&\le (2\pi h)^{-N} \ h^N \int_{Y^h} \Big| \sum_{n\in\mathbb{Z}^N} w^h(n) \ e^{-i2\pi hy\cdot n} \Big|^2 \ dy \\
&\le (2\pi h)^{-N} \ h^N \int_{Y^h} |G^h(y)|^2 \, dy \\
&\le (2\pi h)^{-N} \ \|G^h\|_{L^2_\#(Y^h)}^2 = (2\pi h)^{-N} \ \|w^h\|_{\ell^2}^2 \le \|f^0\|_{L^2(\mathbb{R}^N)}^2
\end{aligned}$$

which proves the asserted bound.

It remains to prove that $f^h \in \mathbb{R}$. Conjugating $\widehat{f^h}$ we get

$$\begin{aligned}
\overline{\widehat{f^h}(y)} &= \sum_{n\in\mathbb{Z}^N} \overline{w^h(n)} \ e^{+i2\pi hy\cdot n} \chi_{|y|\le R^h} \\
&= \sum_{n\in\mathbb{Z}^N} w^h(n) \ e^{-i2\pi h(-y)\cdot n} \chi_{|-y|\le R^h} = \widehat{f^h}(-y)
\end{aligned}$$

since, by Theorem 1, the w_n^h's are real valued. This achieves the proof. $\square$

Let us now show that f^h is not far from satisfying (1).

Lemma 5 *The function f^h satisfies a approximate form of (1) in the sense that*

$$\langle(\partial_t + \xi \cdot \nabla_x) f^h - \Theta(V)(f^h), \varphi\rangle_{\mathcal{S}';\mathcal{S}} = 0$$

holds for all φ in $\mathcal{S}((0,T)\times\mathbb{R}^N\times\mathbb{R}^N)$ with $\operatorname{supp}(\widehat{\varphi}) \subset (0,T)\times\mathbb{R}^N\times B(0,R)$, $0 < R < R^h$.

Proof. Let us set

$$T^h(t,x,n) = (\partial_t + \xi_n \cdot \nabla_x) w^h(t,x,n) - \Theta_d(w^h(t,x,\cdot))(n).$$

One has to compute the action on φ of

$$\mathcal{F}^{-1}_{y\to\xi}\Big(\sum_{n\in\mathbb{Z}^N} e^{-i2\pi hy\cdot n}\ T^h(t,x,n)\ \chi_{|y|\le R^h}\Big).$$

Obviously, there is no difficulty with the time derivative, which commutes with the other operations. It leads to $\partial_t f^h$. Let us consider the Vlasov term. Since, by its definition, f^h has a Fourier transform compactly supported (with respect to the variable y) in $B(0,R^h)$, one has, by Lemma 3-i), $\Theta^h(f^h) = \Theta(f^h)$, with

$$\widehat{\Theta(f^h)}(t,x,y) = i\ D_V(x,y)\ \chi_{|y|\le R^h} \sum_{n\in\mathbb{Z}^N} w^h(t,x,n)\ e^{-i2\pi hy\cdot n}.$$

Let us denote this quantity by $\gamma^h(y)$. It corresponds to

$$\begin{cases} \Gamma^h(t,x,y) = \gamma^h(y) = i\ \mathcal{V}^h(x,y)\ G^h(t,x,y) \quad \text{on } y\in B(0,R^h), \\ \Gamma^h(t,x,y) = 0 \quad \text{on } y \in Y^h\backslash B(0,R^h), \\ \Gamma^h(t,x,y) \quad \text{is } Y^h\text{−periodic (wrt } y). \end{cases}$$

The corresponding Fourier coefficients are therefore given by

$$\widehat{\Gamma^h}(n) = i\ \widehat{\mathcal{V}^h\ G^h}(n) = i\ \widehat{\mathcal{V}^h} * \widehat{G^h}(n) = a^h * w^h(n) = \Theta_d(w^h)(n)$$

by using the definitions of $a^h, \mathcal{V}^h$ and w^h, G^h.

Applying Lemma 1 yields the following equality

$$\begin{aligned} \Theta(f^h) &= \mathcal{F}^{-1}_{y\to\xi}(\gamma^h) = \mathcal{F}^{-1}_{y\to\xi}\Big(\sum_{n\in\mathbb{Z}^N} \widehat{\Gamma^h}(t,x,n)\ e^{-i2\pi hy\cdot n}\ \chi_{|y|\le R^h}\Big) \\ &= \mathcal{F}^{-1}_{y\to\xi}\Big(\sum_{n\in\mathbb{Z}^N} \Theta_d(w^h)(t,x,n)\ e^{-i2\pi hy\cdot n}\ \chi_{|y|\le R^h}\Big), \end{aligned}$$

which is exactly what we need when treating the right hand side of (11). It remains to deal with the convective term. Difficulties could arise due to the truncation $\chi_{|y|\leq R^h}$ in the Fourier variable; however, we have choosen test functions φ that does not feel the action of this operation. Set

$$\begin{aligned} C^h(t,x,y) &= \sum_{n\in\mathbb{Z}^N} e^{-i2\pi hy\cdot n}\ \xi_n\cdot\nabla_x w^h(t,x,n)\ \chi_{|y|\leq R^h} \\ &= (-i)^{-1}\sum_{n\in\mathbb{Z}^N}\nabla_y\nabla_x\big(e^{-i2\pi hy\cdot n}\ w^h(t,x,n)\big)\ \chi_{|y|\leq R^h}\in\mathcal{S}'(\mathbb{R}^+\times\mathbb{R}^N\times\mathbb{R}^N). \end{aligned}$$

We compute, by using the exchange formula,

$$\begin{aligned} \langle\mathcal{F}^{-1}_{y\to\xi}(C^h(t,x,\cdot))(\xi),\varphi\rangle_{\mathcal{S}',\mathcal{S}} &= (2\pi)^{-N}\overline{\langle\mathcal{F}(\overline{C^h}),\varphi\rangle} \\ &= (2\pi)^{-N}\overline{\left\langle\overline{C^h},\mathcal{F}(\overline{\varphi})\right\rangle} \\ &= (2\pi)^{-N}\overline{\left\langle\overline{(-i)^{-1}\nabla_y\nabla_x\big(e^{-i2\pi hy\cdot n}\ w^h(t,x,n)\big)},\mathcal{F}(\overline{\varphi})\right\rangle} \end{aligned}$$

since $\widehat{\varphi}\chi_{|y|\leq R^h}=\widehat{\varphi}$ by using the support assumption. It follows that

$$\begin{aligned} &\langle\mathcal{F}^{-1}_{y\to\xi}(C^h(t,x,\cdot))(\xi),\varphi\rangle_{\mathcal{S}',\mathcal{S}} \\ &\quad=(2\pi)^{-N}\overline{\int\overline{(-i)^{-1}\sum_{n\in\mathbb{Z}^N}e^{-i2\pi hy\cdot n}\ w^h(t,x,n)}\ \nabla_y\nabla_x\mathcal{F}(\overline{\varphi})\,dy\,dx\,dt}. \end{aligned}$$

However, one has

$$\nabla_y\mathcal{F}(\overline{\varphi})=\nabla_y\left(\int_{\mathbb{R}^N}e^{-iy\cdot\xi}\overline{\varphi}(\xi)\,d\xi\right)=-i\mathcal{F}(\xi\overline{\varphi}),$$

which still has its support in $B(0,R^h)$ (with respect to the variable y). Hence, we obtain

$$\begin{aligned} &\langle\mathcal{F}^{-1}_{y\to\xi}(C^h(t,x,\cdot))(\xi),\varphi\rangle_{\mathcal{S}',\mathcal{S}} \\ &\quad=(2\pi)^{-N}\overline{\int\overline{(-i)^{-1}\sum_{n\in\mathbb{Z}^N}e^{-i2\pi hy\cdot n}\ w^h(t,x,n)}\ (-i)\mathcal{F}\big(\xi\cdot\nabla_x\overline{\varphi}\big)\,dy\,dx\,dt}. \end{aligned}$$

We go back with the exchange formula to

$$\begin{aligned} &\langle\mathcal{F}^{-1}_{y\to\xi}(C^h(t,x,\cdot))(\xi),\varphi\rangle_{\mathcal{S}',\mathcal{S}} \\ &\quad=-(2\pi)^{-N}\overline{\langle\mathcal{F}_{y\to\xi}\Big(\overline{\sum_{n\in\mathbb{Z}^N}e^{-i2\pi hy\cdot n}w^h(t,x,n)\chi_{|y|\leq R^h}}\Big)\ ,\ \xi\cdot\nabla_x\overline{\varphi}\rangle} \\ &\quad=\langle\xi\cdot\nabla_x f^h,\varphi\rangle. \end{aligned}$$

This ends the proof of Lemma 5. $\square$

4.2 Convergence

We are now able to establish the convergence of our scheme, which is shown to have spectral accuracy.

Theorem 2 *Assume that f^0 belongs to $H^1(\mathbb{R}^N \times \mathbb{R}^N)$ and $V \in L^\infty(\mathbb{R}^N)$. Let $0 < T < \infty$. Let $f \in C^0(\mathbb{R}^+; L^2(\mathbb{R}^N \times \mathbb{R}^N)) \cap L^\infty(0,T; H^1(\mathbb{R}^N \times \mathbb{R}^N))$ be the associated solution of (1). Let $R^h \leq (2h)^{-1}$, with $2R^h \sim 1/h$ as h goes to 0. Then, one has on the time interval $(0,T)$,*

$$\|(f - f^h)(t)\|_{L^2(\mathbb{R}^N \times \mathbb{R}^N)} \leq C_T \ h,$$

where C_T depends on T and on these H^1 norms.

If, furthermore, $f^0 \in L^2(\mathbb{R}^N_x; H^s(\mathbb{R}^N_\xi))$ with $f \in L^\infty(0,T; L^2(\mathbb{R}^N_x; H^s(\mathbb{R}^N_\xi)))$ and $\nabla_x f \in L^2((0,T) \times \mathbb{R}^N_x; H^{s-1}(\mathbb{R}^N_\xi))$ for some $s > 0$, then the method becomes of order s since one has $\|(f - f^h)(t)\|_{L^2(\mathbb{R}^N \times \mathbb{R}^N)} \leq C_T \ h^s$.

Proof. It would be tempting, in order to derive such an estimate, to multiply the equation satisfied by $f - f^h$ by $\overline{f - f^h}$. However, this function is not an admissible test function in the sense of Lemma 5 since its Fourier transform is not compactly supported. Then, let us introduce a function ζ that fulfills

$$\begin{cases} \zeta(y) = 1 \quad \text{on } B(0,1/2), \qquad \zeta(y) = 0 \quad \text{on } \mathbb{R}^N \backslash B(0,1) \\ 0 \leq \zeta(y) \leq 1, \\ \zeta \in C^1(\mathbb{R}^N). \end{cases}$$

Set $\zeta^h(y) = \zeta(y/R^h)$ and $t^h(t,x,\xi) = \mathcal{F}^{-1}_{y \to \xi}(\widehat{f}(t,x,y)\ \zeta^h(y))$. Mainly, the rate of convergence is determined by the obvious estimate

$$\|f - t^h\|^2_{L^2(\mathbb{R}^N \times \mathbb{R}^N)} = (2\pi)^{-N} \|\widehat{f}(1 - \zeta^h)\|^2_{L^2(\mathbb{R}^N \times \mathbb{R}^N)} \leq \frac{\|f\|^2_{L^2(\mathbb{R}^N_x; H^s(\mathbb{R}^N_\xi))}}{(2\pi)^N (1 + (R^h/2)^2)^s}.$$

Furthermore, let us look at the equation satisfied by t^h: we shall show that it satisfies (1) up to an error term due to the truncation, which can be controlled in $\mathcal{O}(R^h)$ thanks to the H^1 regularity of the solution. From (1), one obtains

$$\partial_t t^h = \mathcal{F}^{-1}(\partial_t \widehat{f}\ \zeta^h) = \mathcal{F}^{-1}(\widehat{\Theta(f)}\ \zeta^h) - \mathcal{F}^{-1}(\widehat{\xi \cdot \nabla_x f}\ \zeta^h).$$

The Vlasov term simply gives

$$\mathcal{F}^{-1}(\widehat{\Theta(f)}\ \zeta^h) = \mathcal{F}^{-1}(D_V\ \widehat{f}\ \zeta^h) = \mathcal{F}^{-1}(D_V\ \mathcal{F}\mathcal{F}^{-1}(\widehat{f}\ \zeta^h)) = \mathcal{F}^{-1}(D_V\ \mathcal{F}(t^h)) = \Theta(t^h).$$

However, error terms are produced by the convective term. Indeed, we have

$$\begin{aligned}
\mathcal{F}^{-1}(\widehat{\xi\cdot\nabla_x f}\ \zeta^h) &= \int_{\mathbb{R}^N} e^{iy\cdot\xi}\ \widehat{\xi\cdot\nabla_x f}(y)\ \zeta^h(y)\,dy/(2\pi)^N \\
&= \int_{\mathbb{R}^N_y} e^{iy\cdot\xi}\left(\int_{\mathbb{R}^N_\eta} e^{-iy\cdot\eta}\ \eta\cdot\nabla_x f(\eta)\,d\eta\right)\zeta^h(y)\,dy/(2\pi)^N \\
&= \int_{\mathbb{R}^N_\eta} \eta\cdot\nabla_x f(\eta)\left(\int_{\mathbb{R}^N_y} e^{iy\cdot(\xi-\eta)}\zeta^h(y)\,dy\right)\,d\eta/(2\pi)^N \\
&= \int_{\mathbb{R}^N_\eta} \eta\cdot\nabla_x f(\eta)\widehat{\zeta^h}(\eta-\xi)\,d\eta/(2\pi)^N \\
&= (\eta\cdot\nabla_x f(\eta) * \check{\widehat{\zeta^h}}(\eta))(\xi)/(2\pi)^N.
\end{aligned}$$

Let us split this expression as follows

$$\mathcal{F}^{-1}(\widehat{\xi\cdot\nabla_x f}\ \zeta^h) = \xi\cdot\nabla_x t^h + E^h$$

where

$$E^h = (\eta\cdot\nabla_x f * \check{\widehat{\zeta^h}}(\eta))(\xi)/(2\pi)^N - \xi\cdot\nabla_x\big(\mathcal{F}^{-1}(\widehat{f}\ \zeta^h)\big).$$

Since

$$\xi\cdot\nabla_x\big(\mathcal{F}^{-1}(\widehat{f}\ \zeta^h)\big) = \int_{\mathbb{R}^N_y} e^{iy\cdot\xi}\zeta^h(y)\xi\cdot\left(\int_{\mathbb{R}^N_\eta} e^{-iy\cdot\eta}\nabla_x f(\eta)\,d\eta\right)\,dy/(2\pi)^N$$

we get

$$\begin{aligned}
E^h &= \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} e^{iy\cdot(\xi-\eta)}(\eta-\xi)\cdot\nabla_x f(\eta)\ \zeta^h(y)\,d\eta\,dy/(2\pi)^N \\
&= \int_{\mathbb{R}^N_\eta} \nabla_x f(\eta)\left(\int_{\mathbb{R}^N_y}(\eta-\xi)e^{iy\cdot(\xi-\eta)}\zeta^h(y)\,dy\right)\,d\eta/(2\pi)^N \\
&= \int_{\mathbb{R}^N_\eta} \nabla_x f(\eta)\left(\frac{1}{i}\int_{\mathbb{R}^N_y} e^{iy\cdot(\xi-\eta)}\nabla_y(\zeta^h(y))\,dy/(2\pi)^N\right)\,d\eta \\
&= \big(\nabla_x f * \mathcal{F}^{-1}_{y\to\xi}(\nabla_y\zeta^h)/i\big)(\xi).
\end{aligned}$$

This produces the estimate

$$\begin{aligned}
\|E^h\|_{L^2(\mathbb{R}^N\times\mathbb{R}^N)} &= (2\pi)^{-N}\|\widehat{\nabla_x f}\ \nabla_y(\zeta^h)\|_{L^2(\mathbb{R}^N\times\mathbb{R}^N)} \\
&\le \|\nabla_x f\|_{L^2(\mathbb{R}^N\times\mathbb{R}^N)}\ \|\nabla_y(\zeta^h)\|_{L^\infty(\mathbb{R}^N)} \\
&\le \|\nabla_x f\|_{L^2(\mathbb{R}^N\times\mathbb{R}^N)}\ \|\nabla_y\zeta\|_{L^\infty(\mathbb{R}^N)}/R^h.
\end{aligned}$$

Therefore, $e^h = t^h - f^h$ has a compactly supported Fourier transform in $B(0, R^h)$ and satisfies, in the sense of Lemma 5

$$(\partial_t + \xi \cdot \nabla_x - \Theta^h)(e^h) = E^h.$$

Standard manipulations lead to the estimate

$$\|e^h(t)\|_{L^2(\mathbb{R}^N\times\mathbb{R}^N)} \leq \|e^h(0)\|_{L^2(\mathbb{R}^N\times\mathbb{R}^N)} + \int_0^t \|E^h\|_{L^2(\mathbb{R}^N\times\mathbb{R}^N)} \leq C_T/R^h,$$

where C_T depens on T, $\|f^0\|_{H^1}$ and $\|f\|_{H^1}$. Now, we can estimate $\|f - f^h(t)\|_{L^2(\mathbb{R}^N\times\mathbb{R}^N)} \leq \|e^h(t)\|_{L^2(\mathbb{R}^N\times\mathbb{R}^N)} + \|f - t^h\|_{L^2(\mathbb{R}^N\times\mathbb{R}^N)} \leq C_T/R^h$, which concludes the proof.

Order s information on f leads to the following slight modification when estimating E^h

$$\begin{aligned}
\|E^h\|^2_{L^2(\mathbb{R}^N\times\mathbb{R}^N)} &= (2\pi)^{-N} \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} |\widehat{\nabla_x f}(y)|^2 \; |\nabla_y(\zeta^h)|^2 \, dy \, dx \\
&\leq (2\pi)^{-N} \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} |\widehat{\nabla_x f}(y)| \; \chi_{|y|\geq R^h/2} \, \frac{1}{(R^h)^2} \; \|\nabla_y \zeta\|^2_{L^\infty(\mathbb{R}^N)} \, dy \, dx \\
&\leq \|\nabla_x f\|^2_{L^2(\mathbb{R}^N_x; H^{s-1}(\mathbb{R}^N_\xi))} \; \|\nabla_y \zeta\|^2_{L^\infty(\mathbb{R}^N)} \; \frac{2 \; (2\pi)^{-N}}{(1+(R^h)^2)^{s-1} \; (R^h)^2}.
\end{aligned}$$

The announced rate of convergence follows easily. □

5 Semi-classical limit

Let us now take into account the (scaled) Planck constant $\varepsilon > 0$. Accordingly, the Wigner operator reads

$$\begin{aligned}
\Theta^\varepsilon(V) f &= \frac{i}{\varepsilon} \mathcal{F}^{-1}_{y\to\xi}\Big(\big(V(x+\varepsilon y/2) - V(x-\varepsilon y/2)\big) \; \widehat{f}(y)\Big) \\
&= \frac{i}{(2\pi)^N} \int_{\mathbb{R}^N} \frac{V(x+\varepsilon y/2) - V(x-\varepsilon y/2)}{\varepsilon} \; \widehat{f}(y) \; e^{iy\cdot\xi} \, dy
\end{aligned}$$

It is a well-established fact that the corresponding sequence $\big(f^\varepsilon\big)_{\varepsilon>0}$ of solutions of the Wigner equation

$$\partial_t f^\varepsilon + \xi \cdot \nabla_x f^\varepsilon = \Theta^\varepsilon(V)(f^\varepsilon)$$

converges, in some weak sense, to a solution F of the Vlasov equation

$$\partial_t F + \xi \cdot \nabla_x F = \nabla_x V \cdot \nabla_\xi F \tag{15}$$

as $\varepsilon \to 0$. We refer to P. L. Lions-Th. Paul [10] for precise statements and rigourous proofs; this can be formally understood from the following facts

$$\begin{cases} i\,\dfrac{V(x+\varepsilon y/2)-V(x-\varepsilon y/2)}{\varepsilon} \longrightarrow i\nabla_x V\cdot y \quad \text{as } \varepsilon\to 0, \\ \widehat{iy} = \nabla\delta_{\xi=0}. \end{cases}$$

Therefore, we would naturally expect that our discrete scheme reproduces this behaviour. Let us first set up some definitions.

Recall that the discrete operator is defined, see (9), by

$$\begin{cases} a_n^{\varepsilon,h} = i\ h^N \displaystyle\int_{\mathbb{R}^N} \frac{V(x+\varepsilon y/2)-V(x-\varepsilon y/2)}{\varepsilon}\,\chi_{|y|\le R^h}(y)\ e^{i2\pi hn\cdot y}\,dy, \\ \Big(\Theta_d^{\varepsilon,h}(V)(w)\Big)_n = (a^{\varepsilon,h}*w)_n = i\widehat{\mathcal{V}^{\varepsilon,h}G^h}(n), \end{cases} \tag{16}$$

where $w(x,n)$ belongs to $L^2(\mathbb{R}^N\times\mathbb{Z}^N)$ and $\mathcal{V}^{\varepsilon,h}(x,\cdot)$ and $G^h(x,\cdot)$ are the Y^h-periodic functions defined on the cell by

$$\begin{cases} \mathcal{V}^{\varepsilon,h}(x,y) = \dfrac{V(x+\varepsilon y/2)-V(x-\varepsilon y/2)}{\varepsilon}\,\chi_{|y|\le R^h}(y) \\ G^h(x,y) = \displaystyle\sum_{n\in\mathbb{Z}^N} w(x,n)\ e^{-i2\pi hn\cdot y}. \end{cases}$$

For small ε, one expects that $\Theta_d^{\varepsilon,h}$ looks like the following discrete operator

$$\Big(\mathbb{V}^h(V)(w)\Big)_n = (u^h*w)_n = i\widehat{\mathcal{Y}^hG^h}(n), \tag{17}$$

where $\mathcal{Y}^h(x,\cdot)$ is the Y^h-periodic function given by

$$\mathcal{Y}^h(x,y) = \nabla_x V(x)\cdot y\ \chi_{|y|\le R^h}(y)$$

for $x\in\mathbb{R}^N$ and $y\in Y^h$. This discrete operator corresponds to our interpretation of the Vlasov term $\nabla_x V\cdot\nabla_\xi g$ when reasoning as in Section 2 for a function g with $\widehat{g}$ compactly supported in $B(0,R)$. One remarks that

$$u_n^h = i\int_{\mathbb{R}^N} \nabla_x V(x)\cdot y\ \chi_{|y|\le R^h}(y)\ e^{i2\pi hn\cdot y}\,dy = \overline{u_n^h} = -u_{-n}^h$$

so that the coefficients are real and even; in turn, $\mathbb{V}^h$ is a skew-symmetric operator of $\mathcal{L}(\ell^2)$ for $h>0$ fixed and $V\in W^{1,\infty}(\mathbb{R}^N)$. Hence, reproducing the arguments of the proof of Theorem 1, we show that the corresponding discrete problem is well-posed.

Theorem 3 *Let $v^{h,0} \in L^2(\mathbb{R}^N_x \times \mathbb{Z}^N_n)$ and $V \in W^{1,\infty}(\mathbb{R}^N)$. The problem*

$$\left\{ \begin{array}{ll} \partial_t v_n + \xi_n \cdot \nabla_x v_n = \mathbb{V}^h(V)(v)_n & \text{in } \mathbb{R}^+_t \times \mathbb{R}^N_x \times \mathbb{Z}^N_n \\ v_{|t=0} = v^0 & \end{array} \right. \tag{18}$$

has a unique mild solution $v^h \in C^0([0,T]; L^2(\mathbb{R}^N_x \times \mathbb{Z}^N))$. Furthermore, if the initial data $v^{h,0}$ is real valued (i.e. $v^{h,0}(x,n) = \overline{v^{h,0}(x,n)}$ for all $n \in \mathbb{Z}^N$ and a. a. $x \in \mathbb{R}^N$) then, the solution v^h remains real valued and the relation $\|v^h(t)\|_{L^2(\mathbb{R}^N \times \mathbb{Z}^N)} = \|v^{h,0}\|_{L^2(\mathbb{R}^N \times \mathbb{Z}^N)}$ holds.

Let us denote, according to Section 4,

$$\left\{ \begin{array}{l} f^{\varepsilon,h}(t,x,\xi) = \mathcal{F}^{-1}_{y \to \xi}\Big(\displaystyle\sum_{n \in \mathbb{Z}^N} w^{\varepsilon,h}(t,x,n)\ e^{-i2\pi h y \cdot n}\ \chi_{|y| \le R^h} \Big), \\ F^h(t,x,\xi) = \mathcal{F}^{-1}_{y \to \xi}\Big(\displaystyle\sum_{n \in \mathbb{Z}^N} v^h(t,x,n)\ e^{-i2\pi h y \cdot n}\ \chi_{|y| \le R^h} \Big), \end{array} \right.$$

where $w^{\varepsilon,h}$, and v^h are the solutions of (11) and (18), respectively, obtained from well-prepared initial data as in Lemma 4. We naturally assume in this construction that $f^{\varepsilon,0}(x,\xi)$, which defines $w^{\varepsilon,h}_{t=0}$, tends (strongly in $L^2(\mathbb{R}^N \times \mathbb{R}^N)$) to $F^0(x,\xi)$, associated to $v^h_{t=0}$, when $\varepsilon \to 0$. Of course, we wish to justify the following diagramm

$$\begin{array}{ccc} \begin{array}{l} w^{\varepsilon,h},\ f^{\varepsilon,h} \\ \text{discrete Wigner} \end{array} & \xrightarrow{\ h \to 0\ } & \begin{array}{l} f^{\varepsilon} \\ \text{continuous Wigner} \end{array} \\ \Big\downarrow \varepsilon \to 0 & & \Big\downarrow \varepsilon \to 0,\ [10] \\ \begin{array}{l} v^h,\ F^h \\ \text{discrete Vlasov} \end{array} & \xrightarrow[\ h \to 0\ ]{} & \begin{array}{l} F \\ \text{continuous Vlasov} \end{array} \end{array}$$

Obviously, Lemma 4 adapts to the scaling.

Lemma 6 *We have*

$$\begin{array}{l} \|w^{\varepsilon,h}(t)\|^2_{L^2(\mathbb{R}^N \times \mathbb{Z}^N)} \le (2\pi h)^N\ \|f^{\varepsilon,0}\|^2_{L^2(\mathbb{R}^N \times \mathbb{R}^N)} \le (2\pi h)^N\ C_0, \\ \|v^h(t)\|^2_{L^2(\mathbb{R}^N \times \mathbb{Z}^N)} \le (2\pi h)^N\ \|F^0\|^2_{L^2(\mathbb{R}^N \times \mathbb{R}^N)}, \end{array}$$

and the (real valued) sequences $\left(F^h\right)_{h>0}$, $\left(f^{\varepsilon,h}\right)_{\varepsilon>0,h>0}$ are bounded in $L^\infty(\mathbb{R}^+, L^2(\mathbb{R}^N \times \mathbb{R}^N))$, uniformly with respect to ε and h.

Next, the strategy developped in the proof of Lemma 5 and Theorem 2 applies when dealing with v^h, F^h and we are led to the following statement.

Theorem 4 *Let $V \in W^{1,\infty}(\mathbb{R}^N)$. The function F^h satisfies a approximate form of (15) in the sense that*

$$\langle(\partial_t + \xi \cdot \nabla_x)F^h - \nabla_x V \cdot \nabla_\xi F^h, \varphi\rangle_{\mathcal{S}';\mathcal{S}} = 0$$

holds for all φ in $\mathcal{S}((0,T) \times \mathbb{R}^N \times \mathbb{R}^N)$ with $\operatorname{supp}(\widehat{\varphi}) \subset (0,T) \times \mathbb{R}^N \times B(0,R)$, $0 < R < R^h$.

Assume that F^0 belongs to $H^1(\mathbb{R}^N \times \mathbb{R}^N)$. Let $0 < T < \infty$. Let $F \in C^0(\mathbb{R}^+; L^2(\mathbb{R}^N \times \mathbb{R}^N)) \cap L^\infty(0,T; H^1(\mathbb{R}^N \times \mathbb{R}^N))$ be the associated solution of (15). Let $R^h \le (2h)^{-1}$, with $2R^h \sim 1/h$ as h goes to 0. Then, one has on the time interval $(0,T)$,

$$\|(F - F^h)(t)\|_{L^2(\mathbb{R}^N \times \mathbb{R}^N)} \le C_T\ h,$$

where C_T depends on T and on these H^1 norms.

If, furthermore, $F^0 \in L^2(\mathbb{R}^N_x; H^s(\mathbb{R}^N_\xi))$ with $F \in L^\infty(0,T; L^2(\mathbb{R}^N_x; H^s(\mathbb{R}^N_\xi)))$ and $\nabla_x F \in L^2((0,T) \times \mathbb{R}^N_x; H^{s-1}(\mathbb{R}^N_\xi))$ for some $s > 0$, then the method becomes of order s since one has $\|(F - F^h)(t)\|_{L^2(\mathbb{R}^N \times \mathbb{R}^N)} \le C_T\ h^s$.

We are left with the task of studying the behaviour of $w^{\varepsilon,h}$ as $\varepsilon \to 0$. The convergence to the solution of the discrete Vlasov equation will be a consequence of the following claim.

Proposition 2 *Let $V \in C^1 \cap W^{1,\infty}(\mathbb{R}^N)$. The sequence of operators $\Theta_d^{\varepsilon,h}$ converges strongly to $\mathbb{V}^h$: for any $h > 0$ and $w \in L^2(\mathbb{R}^N \times \mathbb{Z}^N)$, one has*

$$\lim_{\varepsilon \to 0} \|\Theta_d^{\varepsilon,h}(w) - \mathbb{V}^h(w)\|_{L^2(\mathbb{R}^N \times \mathbb{Z}^N)} = 0.$$

Proof. We simply remark that

$$\mathcal{V}^{\varepsilon,h}(x,y) - \mathcal{Y}^h(x,y) = \int_0^1 \Big(\nabla_x V(x + \varepsilon y(\theta - 1/2)) - \nabla_x V(x)\Big) \cdot y\ \chi_{|y| \le R^h}(y)\, d\theta$$

Since $\nabla_x V$ is continuous and bounded, we can apply the Lebesgue theorem which yields for $h > 0$, $x \in \mathbb{R}^N$, $y \in Y^h$,

$$\lim_{\varepsilon \to 0} \big(\mathcal{V}^{\varepsilon,h}(x,y) - \mathcal{Y}^h(x,y)\big) = 0,$$

with the domination $|\mathcal{V}^{\varepsilon,h}(x,y)-\mathcal{Y}^h(x,y)|\leq 2\|\nabla_x V\|_{L^\infty(\mathbb{R}^N)}R^h$. Therefore, one deduces that

$$\begin{array}{rcl} \|\Theta_d^{\varepsilon,h}(w)-\mathbb{V}^h(w)\|^2_{L^2(\mathbb{R}^N\times\mathbb{Z}^N)} & = & \|(\mathcal{V}^{\varepsilon,h}-\mathcal{Y}^h)G^h\|^2_{L^2(\mathbb{R}^N;L^2(Y^h))} \\ & = & h^N\displaystyle\int_{\mathbb{R}^N}\int_{Y^h}\left|\mathcal{V}^{\varepsilon,h}(x,y)-\mathcal{Y}^h(x,y)\right|^2\,|G^h(x,y)|^2\,dy\,dx \\ & \longrightarrow & 0 \end{array}$$

as $\varepsilon\to 0$, still by using the Lebesgue theorem. □

Theorem 5 *As ε goes to 0, the following convergences hold*

$$\left\{\begin{array}{l} \lim\limits_{\varepsilon\to 0}\|w^{\varepsilon,h}-v^h\|_{L^\infty(0,T;L^2(\mathbb{R}^N\times\mathbb{Z}^N))}=0, \\ \lim\limits_{\varepsilon\to 0}\|f^{\varepsilon,h}-F^h\|_{L^\infty(0,T;L^2(\mathbb{R}^N\times\mathbb{R}^N))}=0. \end{array}\right.$$

Proof. It suffices to establish the convergence at the discrete level since the second follows easily (see the proof of Corollary 1). Set $e^{\varepsilon,h}(t,x,n)=w^{\varepsilon,h}(t,x,n)-v^h(t,x,n)$ which satisfies

$$\partial_t e_n^{\varepsilon,h}+\xi_n\cdot\nabla_x e_n^{\varepsilon,h}-\Theta_d^{\varepsilon,h}(V)(e^{\varepsilon,h})_n=\left[\left(\mathbb{V}^h-\Theta_d^{\varepsilon,h}(V)\right)v^h\right]_n.$$

Multiplying by $\overline{e^{\varepsilon,h}}$ and using that $\Theta_d^{\varepsilon,h}$ is skew-symmetric lead to the estimate

$$\|e^{\varepsilon,h}(t)\|_{L^2(\mathbb{R}^N\times\mathbb{Z}^N)}\leq\|e^{\varepsilon,h}(0)\|_{L^2(\mathbb{R}^N\times\mathbb{Z}^N)}+\int_0^t\|(\Theta_d^{\varepsilon,h}-\mathbb{V}^h)v^h(s)\|_{L^2(\mathbb{R}^N\times\mathbb{Z}^N)}\,ds$$

that tends to 0 when $\varepsilon\to 0$ by Proposition 2 and the hypothesis made on the initial data. □

As a concluding remark, let us show that the Vlasov equation can still be obtained from the discrete model when $\varepsilon,h\to 0$ together. Indeed, $f^{\varepsilon,h}$ satisfies a uniform L^2 estimate, see Lemma 6. Then, up to a subsequence, we can suppose that it has a weak limit

$$f^{\varepsilon,h}\rightharpoonup g\qquad\text{weakly}-*\text{ in }L^\infty(0,T;L^2(\mathbb{R}^N\times\mathbb{R}^N)).$$

Multiplying by a test function $\varphi\in\mathcal{S}(\mathbb{R}\times\mathbb{R}^N\times\mathbb{R}^N)$ with $\mathrm{supp}(\widehat{\varphi})\subset(0,T)\times\mathbb{R}^N\times B(0,R)$, $0<R<R^h$, one has the formula of Lemma 5

$$\langle(\partial_t+\xi\cdot\nabla_x)f^{\varepsilon,h},\varphi\rangle_{\mathcal{S}';\mathcal{S}}=\langle f^{\varepsilon,h},\Theta^{\varepsilon,*}(V)\varphi\rangle_{\mathcal{S}';\mathcal{S}}.$$

When $\varepsilon, h \to 0$ the weak convergence of $f^{\varepsilon,h}$ combines to the strong convergence $\Theta^{\varepsilon,*}(V)\varphi \to -\nabla_x V \cdot \nabla_\xi \varphi$ in L^2 and we get

$$\langle (\partial_t + \xi \cdot \nabla_x) g - \nabla_x V \cdot \nabla_\xi g, \varphi \rangle_{\mathcal{S}';\mathcal{S}} = 0,$$

for any $\varphi \in \mathcal{S}$ whose Fourier transform is compactly supported. However the set of admissible test functions is dense in $\mathcal{S}$, so that one deduces that g actually solves the Vlasov equation.

Theorem 6 *When ε, h tend to 0 together, the sequence $f^{\varepsilon,h}$ converges weakly in $L^2((0,T) \times \mathbb{R}^N \times \mathbb{R}^N)$ to a solution of the Vlasov equation.*

References

[1] Arnold A., Lange H. and Zweifel P., *A discrete-velocity stationary Wigner equation*, Preprint.

[2] Arnold, A. and Ringhofer, C., *An operator splitting method for the Wigner-Poisson problem*, SIAM J. Numer. Anal., 33, 1622-1643 (1996).

[3] Degond P. and Markowich P., *A quantum-transport model for semiconductors: the Wigner-Poisson problem for a bounded Brillouin zone*, M2AN, 24, 697-710 (1990).

[4] Gérard, P., Markowich, P., Mauser, N. and Poupaud, F., *Homogenization limits and Wigner transforms*, Comm. Pure Appl. Math. 50, no. 4, 323-379 (1997) and Comm. Pure Appl. Math. 53, no. 2, 280-281 (2000).

[5] Markowich, P., *On the equivalence of the Schrödinger and the quantum Liouville equations*, Math. Methods Appl. Sci. 11, no. 4, 459-469 (1989).

[6] Markowich P., Pietra P. and Pohl C., *Numerical approximation of quadratic observables of Schrödinger-type equations in the semi-classical limit*, Numer. Math., 81, 595-630 (1999).

[7] Markowich P. and Poupaud F., *The pseudo-differential approach to finite-difference revisited*, Calcolo, 36, 161-186 (1999).

[8] Markowich, P. and Ringhofer, C., *An analysis of the quantum Liouville equation*, Z. Angew. Math. Mech. 69, no. 3, 121-127 (1989).

[9] Markowich, P., Ringhofer, C. and Schmeiser, C., **Semiconductor equations** (Springer-Verlag, 1990).

[10] Lions P.-L. and Paul Th., *Sur les mesures de Wigner*, Rev. Mat. Ib., 9, 553-618 (1993).

[11] Ringhofer C., *Computational methods for semiclassical and quantum transport in semiconductor devices*, Acta Numerica, 6, 485-521 (1997).

[12] Ringhofer C., *A spectral collocation technique for the solution of the Wigner-Poisson problem*, SIAM J. Numer. Anal., 29, 679-700 (1992).

[13] Ringhofer C., *On the convergence of spectral methods for the Wigner-Poisson problem*, Math. Models Methods Appl. Sc., 2, 91-112 (1991).

[14] Wigner E., *On the quantum correction to thermodynamic equilibrium*, Phys. Rev., 40, 742-759 (1932).