

# Convergence of Semi-discrete Stationary Wigner Equation with Inflow Boundary Conditions

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## Abstract

Making use of the Whittaker-Shannon interpolation formula with shifted sampling points, we propose in this paper a well-posed semi-discretization of the stationary Wigner equation with inflow BCs. The convergence of the solutions of the discrete problem to the continuous problem is then analysed, providing certain regularity of the solution of the continuous problem.

**Keywords:** Stationary Wigner equation, inflow boundary conditions, well-posedness.

**AMS subject classifications:** 35Q40, 65N35

## 1 Introduction

The Wigner equation is one of the quantum frameworks equivalent to the Schrödinger equation in some sense. The Wigner function is a quasi-probability distribution introduced by Wigner in 1932 to study quantum corrections to classical statistical mechanics [21]. A great many applications of the Wigner equation arose in pervasive fields, including statistical mechanics, quantum optics, quantum chemistry, etc. Particularly, in the simulation of nano-scale semiconductor devices, the Wigner equation was regarded as a promising tool since it is the counterpart of the Boltzmann equation in quantum mechanics. In 1987, Frensley [4] numerically solved the stationary Wigner equation with inflow boundary condition and successfully reproduced the negative differential resistance phenomenon, which is a typical quantum effect verified by experiments. This work motivated a lot of later work on numerical simulations based on the Wigner equation [9, 20, 19, 5, 16, 18, 12]. In these work, different boundary conditions are proposed for the stationary Wigner equation, e.g., absorbing boundary conditions [1] and device adaptive inflow boundary conditions [10]. Among these boundary conditions, the inflow boundary condition is the most popular one due to its simplicity.

In spite of its popularity, the Wigner equation with inflow boundary conditions (BCs) is far from thoroughly studied from a mathematical point of view. Numbers of mathematicians were then attracted to the study of the Wigner equation with inflow BCs, while

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there are seldom results on the well-posedness of the problem yet. For the time-dependent Wigner equation with inflow BCs, well-posedness has been studied for the linear case [14] and the nonlinear case [13], respectively. To the authors knowledge, only one study has been carried out on the stationary Wigner equation, where a rather involved technical method was used to construct a solution [11]. The stationary problem is even interesting since it is applied to the current-voltage curve computation of semiconductor devices in nano-scale, while a rigid proof of the unique solvability has not yet been given. On the other hand, there are comparatively fruitful studies in the numerical approximation aspect. The well-posedness of the semi-discrete stationary Wigner equation with inflow BCs has been proved in [2] if the velocity interval centered at zero is neglected. The numerical convergence for the initial value problem has been studied for the transient Wigner equation [17, 3, 6]. Using the Whittaker-Shannon interpolation formula, Goudon in [6] constructed a converge sequence, which are the solution of a semi-discrete version of the Wigner equation, to approximate the solution of the transient Wigner equation, in case that there exists a unique smooth solution of the continuous problem.

Motivated by the work in [2] and [6], we consider in this paper the convergence of the semi-discrete solution of the stationary Wigner equation with the inflow BCs. The Whittaker-Shannon interpolation formula in [6] is not able to be applied to stationary problem, since it results in a singular semi-discrete problem. We introduce a shift of the sampling points in the Whittaker-Shannon interpolation formula thus the zero velocity is excluded from the sampling points. Thus, the technique in [2] is applicable to prove the well-posedness of the semi-discrete problem we propose. The well-posedness of the semi-discrete equation makes us able to analyze the convergence of the solutions of the semi-discrete problem to the continuous problem. It is proved that the convergence rate depends only on the data and the regularity of the solution of the continuous problem. As a necessary condition for any numerical method, the well-posedness of the continuous problem definitely has to be assumed, which provides us a solution with certain regularity thus the numerical approximation is possible.

The rest part of this paper is arranged as follows. In Section 2, we give the semi-discretization of the stationary Wigner equation with inflow BCs based on Whittaker-Shannon interpolation formula using shifted sampling points. In Section 3, we give an estimate to the semi-discrete residual of the discretization as a preparation to the final convergence result. In Section 4, the convergence of the solution of the semi-discrete problem to the continuous problem is clarified. The Whittaker-Shannon interpolation formula with shifted sampling points is collected in the appendix for reference.

## 2 Discretization

We are considering the stationary dimensionless Wigner equation [21]

$$v \frac{\partial f(x, v)}{\partial x} - \Theta[V](f) = 0, \quad (2.1)$$

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

$$\Theta[V](f)(x, v) = i\mathcal{F}_{y \rightarrow v}^{-1} (D_V(x, y) \mathcal{F}_{v \rightarrow y} (f(x, v))), \quad (2.2)$$

where  $D_V(x, y) = V(x+y/2) - V(x-y/2)$  and  $V(x)$  is the potential. The Fourier transform of  $u(v)$  and its inverse are standard as

$$\widehat{u}(y) = \mathcal{F}_{v \rightarrow y}(u(v)) = \int_{\mathbb{R}} u(v) e^{-ivy} dy,$$

and

$$u(v) = \mathcal{F}_{y \rightarrow v}^{-1}(\widehat{u}(y)) = \frac{1}{2\pi} \int_{\mathbb{R}} \widehat{u}(y) e^{ivy} dy.$$

According to the convolution theorem of the Fourier transform, the pseudo-differential operator defined in (2.2) can be written into

$$\Theta[V](f) = \mathcal{V}(x, \cdot) * f(x, \cdot) = \int_{\mathbb{R}} \mathcal{V}(x, v - v') f(x, v') dv',$$

where the Wigner potential  $\mathcal{V}(x, v)$  is related to the potential  $V(x)$  through

$$\mathcal{V}(x, v) = i\mathcal{F}_{y \rightarrow v}^{-1}(D_V(x, y)) = \frac{i}{2\pi} \int_{-\infty}^{\infty} D_V(x, y) e^{ivy} dy. \quad (2.3)$$

Then the Wigner equation is reformulated as

$$v \frac{\partial f(x, v)}{\partial x} - \int_{v' \in \mathbb{R}} \mathcal{V}(x, v - v') f(x, v') dv' = 0, \quad (x, v) \in (0, l) \times \mathbb{R}, \quad (2.4)$$

subject to the inflow boundary condition

$$f(0, v) = f_b(v), \quad \text{if } v > 0, \quad f(l, v) = f_b(v), \quad \text{if } v < 0. \quad (2.5)$$

We apply the Fourier transform to the Wigner equation (2.4) and obtain

$$i \frac{\partial^2}{\partial x \partial y} \widehat{f}(x, y) - i D_V(x, y) \widehat{f}(x, y) = 0. \quad (2.6)$$

We introduce a smooth cutoff function  $\zeta_h(y) \in C_0^\infty(\mathbb{R})$  as in [7] satisfying

$$\zeta_h(y) = \zeta(y/R^h), \quad R^h = \frac{1}{2h} \quad (2.7)$$

and

$$\begin{cases} 0 \leq \zeta(y) \leq 1, \\ \zeta(y) = \begin{cases} 1, & \text{on } B(0, 1/2), \\ 0, & \text{on } \mathbb{R} \setminus B(0, 3/4). \end{cases} \end{cases}$$

And it is easy to see that

$$\zeta_h'(y) = 0, \quad \text{if } |y| \notin \left[ \frac{R^h}{2}, \frac{3R^h}{4} \right]. \quad (2.8)$$

Furthermore, the derivative of the cutoff function  $\zeta_h(y)$  [7] may satisfy

$$|\zeta_h'(y)| \leq C_\zeta h, \quad \forall y \in \mathbb{R}, \quad (2.9)$$

where  $C_\zeta$  is a constant independent of  $h$ . Multiplying  $\zeta_h(y)$  on both sides of (2.6) yields

$$\zeta_h(y) \frac{\partial^2}{\partial x \partial y} \widehat{f}(x, y) - \zeta_h(y) D_V(x, y) \widehat{f}(x, y) = 0. \quad (2.10)$$

Thus we have

$$\frac{\partial^2}{\partial x \partial y} (\widehat{f}(x, y) \zeta_h(y)) - D_V(x, y) \widehat{f}(x, y) \zeta_h(y) = \frac{\partial}{\partial x} (\widehat{f}(x, y) \zeta_h'(y)). \quad (2.11)$$

Let

$$t^h(x, v) = \mathcal{F}_{y \rightarrow v}^{-1} (\widehat{f}(x, y) \zeta_h(y)),$$

which is a function with a compactly supported Fourier transform, precisely  $\text{supp}(\widehat{t^h}(x, y)) \subset \text{supp}(\zeta_h(y)) \subset B(0, \frac{3}{4}R^h)$ . According to the Shannon sampling theory,  $t^h(x, v)$  can be completely represented by the Whittaker-Shannon interpolation formula (A.1)

$$t^h(x, v) = \sum_{n \in \mathbb{Z}} t^h(x, v_n) \text{sinc} \left( R^h(v - v_n) \right), \quad (2.12)$$

where  $v_n = (n + 1/2) \frac{\pi}{R^h}$ .

We then apply the inverse Fourier transform to (2.11) to yield the equation of  $t^h(x, v)$

$$v \frac{\partial}{\partial x} t^h(x, v) - \Theta[V] t^h(x, v) = \mathcal{T}^h(x, v),$$

where

$$\widehat{\mathcal{T}^h}(x, y) = \frac{\partial}{\partial x} \widehat{f}(x, y) \zeta_h'(y).$$

By Lemma 5, we have that  $\Theta[V] t^h(x, v) = \Theta[V \chi_{B(0, R^h)}] t^h(x, v)$  due to (A.2), thus

$$v \frac{\partial}{\partial x} t^h(x, v) - \Theta[V \chi_{B(0, R^h)}] t^h(x, v) = \mathcal{T}^h(x, v). \quad (2.13)$$

By setting  $v = v_n$  in (2.13), we have

$$v_n \frac{dt^h(x, v_n)}{dx} - (\Theta[V \chi_{B(0, R^h)}] t^h)(x, v_n) = \mathcal{T}^h(x, v_n), \quad n \in \mathbb{N}. \quad (2.14)$$

The Shannon sampling theorem tells one that (2.13) is equivalent to the discrete-velocity equations (2.14). We point out that

$$(\Theta[V \chi_{B(0, R^h)}] t^h)(x, v_n) = \frac{\pi}{R^h} \sum_{m \in \mathbb{Z}} \tilde{\mathcal{V}}_{n-m} t^h(x, v_m),$$

where  $\tilde{\mathcal{V}}_n(x)$  is defined by

$$\tilde{\mathcal{V}}_n(x) = \frac{i}{2\pi} \int_{B(0, R^h)} D_V(x, y) e^{iy n \frac{\pi}{R^h}} dy,$$

and it is equal to the inverse Fourier transform of the truncated function  $i D_V(x, y) \chi_{B(0, R^h)}$  at velocity  $\tilde{v}_n = n\pi/R^h$

$$\tilde{\mathcal{V}}_n(x) = i \mathcal{F}_{y \rightarrow v}^{-1} \left( D_V(x, y) \chi_{B(0, R^h)}(y) \right) (\tilde{v}_n). \quad (2.15)$$

This allows us to reformulate (2.14) as

$$v_n \frac{dt^h(x, v_n)}{dx} - \frac{\pi}{R^h} \sum_{m \in \mathbb{Z}} \tilde{\mathcal{V}}_{n-m} t^h(x, v_m) = \mathcal{T}^h(x, v_n), \quad n \in \mathbb{N}.$$

A reasonable problem one may be interested in is the case that  $\mathcal{T}^h(x, v)$  goes to zero as  $h \rightarrow 0$ . As a special setup, if  $\hat{f}(x, y)$  has a compact support in  $B(0, R^h/2)$ , then  $\mathcal{T}^h(x, v) = 0$ . Hence we are motivated to propose the semi-discrete version of the Wigner equation as

$$v_n \frac{df_n(x)}{dx} - \frac{\pi}{R^h} \sum_{m \in \mathbb{Z}} \tilde{\mathcal{V}}_{n-m} f_m(x) = 0, \quad (2.16)$$

subject to

$$f_n(0) = t_b^h(v_n), \text{ if } n \geq 0, \quad f_n(l) = t_b^h(v_n), \text{ if } n < 0, \quad (2.17)$$

where

$$t_b^h(v) = \mathcal{F}_{y \rightarrow v} (\mathcal{F}_{v \rightarrow y}^{-1} (f_b(v)) \zeta_h(y)).$$

This is formulated as a boundary value problem (BVP). Since  $v = 0$  is excluded from the sampling points  $v_n$ , the method to prove the well-posedness of the semi-discrete Wigner equation with inflow boundary conditions in [2] is then applicable to the BVP (2.16)-(2.17). Here we directly conclude that the BVP (2.16)-(2.17) admits a unique solution  $f_n(x)$ .

We let

$$f^h(x, v) = \sum_n f_n(x) \text{sinc} \left( R^h(v - v_n) \right), \quad (2.18)$$

as the approximation of  $t^h(x, v)$ . If there is a fast enough decay of  $\hat{f}(x, y)$  in terms of  $y$ , the residual term  $\mathcal{T}^h(x, v)$  can be arbitrary small as  $h$  going to zero. With a small enough residual  $\mathcal{T}^h(x, v)$ , not only the difference of  $f^h(x, v)$  from  $t^h(x, v)$  is small, but also the difference between  $t^h(x, v)$  and  $f(x, v)$  may be small. Consequently, it is expected that  $f^h(x, v)$  is an appropriate approximation of the continuous problem if there is a fast enough decay of  $\hat{f}(x, y)$  in terms of  $y$ . The major object in the rest of this paper is to give the precise senses of this conclusion and its rigid proof.

### 3 Estimate of Semi-discrete Residual

We denote the semi-discrete residual to be  $e_n^h(x) = t^h(x, v_n) - f_n(x)$ . Comparing (2.14) and (2.16), we have the equation for  $e_n^h(x)$

$$v_n \frac{de_n^h(x)}{dx} - \frac{\pi}{R^h} \sum_m \tilde{\mathcal{V}}(x, v_n - v_m) e_m^h(x) = \mathcal{T}^h(x, v_n). \quad (3.1)$$

Clearly we have  $e_n^h(0) = 0$  for  $n \geq 0$  and  $e_n^h(l) = 0$  for  $n < 0$  since the inflow BCs of  $f_n^h(x)$  and  $t^h(x, v_n)$  are the same. This is again a BVP, while it is nonhomogeneous. We directly extend the method in [2] to this nonhomogeneous BVP to give an upper bound estimate, which is used to prove the convergence of the approximate solution.

At first, let us introduce the notations used in [2]. From the discrete equation (3.1) of  $e_n^h$ , we introduce vector functions  $\mathbf{e}^h = \{e_n^h\}_{n \in \mathbb{Z}}$ ,  $\mathbf{T}^h = \{\mathcal{T}_n^h\}_{n \in \mathbb{Z}}$ , then we have

$$\mathbf{T} \frac{d\mathbf{e}^h(x)}{dx} - \mathbf{A}(x) \mathbf{e}^h = \mathbf{T}^h \quad (3.2)$$

with the BCs

$$\begin{cases} \mathbf{e}_n^h(0) = 0, n \geq 0, \\ \mathbf{e}_n^h(l) = 0, n < 0, \end{cases} \quad (3.3)$$

where  $\mathbf{T}$  and  $\mathbf{A}(x)$  are defined as

$$\mathbf{T} = \text{diag}(v_n)_{n \in \mathbb{Z}}, \quad \mathbf{A}(x) = \left( \frac{\pi}{R^h} \tilde{\mathcal{V}}(x, v_n - v_m) \right)_{n, m \in \mathbb{Z}}. \quad (3.4)$$

We show below that for  $0 \leq x \leq l$ ,  $\mathbf{A}(x)$  is a bounded linear operator on  $H := l^2$  and  $x \rightarrow \mathbf{A}(x)$  is continuous in the uniform operator topology. Here  $l^2$  is the real Hilbert space with natural inner product  $(\mathbf{x}, \mathbf{y}) = \sum_{n \in \mathbb{Z}} x_n y_n$ . Notice that  $\mathbf{A}(x)$  is a representation based on sampling points of  $\Theta[V\chi_B(0, R^h)]$  on  $X^h = \{e^h(x, v) \in L^2(\mathbb{R}_v) : \hat{e}^h(x, y) \subset B(0, R^h)\}$ . According to Shannon sampling theory,  $\|e^h(x, v)\|_{L^2(\mathbb{R}_v)}^2 = \frac{\pi}{R^h} \|\mathbf{e}^h\|_{l^2}^2$ . So  $\mathbf{e}^h \in l^2$  implies  $e^h(x, v) \in X^h$ . By Lemma 5, we can conclude that  $\mathbf{A}(x)$  can be defined as

$$(\mathbf{A}(x)\mathbf{e}^h)_n = (\Theta[V\chi_{B(0, R^h)}]e^h)(x, v_n).$$

Thus we have

$$\frac{\pi}{R^h} \|\mathbf{A}(x)\mathbf{e}^h\|_{l^2}^2 = \|(\Theta[V\chi_{B(0, R^h)}]e^h)(x, \cdot)\|_{L^2(\mathbb{R}_v)}^2.$$

According to Parseval's theorem of the Fourier transform, we have

$$\frac{\pi}{R^h} \|\mathbf{A}(x)\mathbf{e}^h\|_{l^2}^2 = \frac{1}{2\pi} \|D_V(x, y)\chi_{B(0, R^h)}\hat{e}^h(x, y)\|_{L^2(\mathbb{R}_y)}^2 \leq 4\|V\|_{L^\infty}^2 \frac{\pi}{R^h} \|\mathbf{e}^h\|_{l^2}^2.$$

Thus the norm of  $\mathbf{A}(x)$  is uniformly bounded by

$$\|\mathbf{A}(x)\| \leq 2\|V\|_{L^\infty}, \quad (3.5)$$

and  $\mathbf{A} \in L^1((0, l); B(H))$ , where  $B(\cdot)$  is the space of linear operator on a Hilbert space.

Following [2], we need to transform it into an initial value problem (IVP) using the technique therein. At first, we denote  $\mathbb{Z}^- = \{n \in \mathbb{Z} : n < 0\}$  and  $\mathbb{Z}^+ = \{n \in \mathbb{Z} : n \geq 0\}$ .  $H$  may be decomposed as  $H = H^- \oplus H^+$  where  $H^\pm = l^2(\mathbb{Z}^\pm)$ . We denote by  $Q^\pm$  the restrictions of  $H$  onto  $H^\pm$ , i.e.,  $Q^\pm \mathbf{e}^h = \mathbf{e}^{h^\pm}$  for any  $\mathbf{e}^h = (\mathbf{e}^{h^+}, \mathbf{e}^{h^-})$ ,  $\mathbf{e}^{h^\pm} \in H^\pm$ . Let  $P^\pm$  be the projections defined by  $P^+ \mathbf{e}^h = (0, \mathbf{e}^{h^+})$ ,  $P^- \mathbf{e}^h = (\mathbf{e}^{h^-}, 0)$ , and the embeddings  $E^\pm : H^\pm \rightarrow H$  are defined by  $E^+ \mathbf{e}^{h^+} = (0, \mathbf{e}^{h^+})$ ,  $E^- \mathbf{e}^{h^-} = (\mathbf{e}^{h^-}, 0)$ . One has the relations that  $P^\pm = E^\pm Q^\pm$ .

Since  $\mathbf{A}$  is clearly skew-symmetric, it is decomposed as

$$\mathbf{A}(x) = \begin{pmatrix} \mathbf{A}^{--} & \mathbf{A}^{-+} \\ \mathbf{A}^{+-} & \mathbf{A}^{++} \end{pmatrix} = -\mathbf{A}^*(x) \quad (3.6)$$

with  $\mathbf{A}^{++} = Q^+ \mathbf{A} E^+ \in B(H^+)$ ,  $\mathbf{A}^{+-} = Q^+ \mathbf{A} E^- \in B(H^-, H^+)$ ,  $\mathbf{A}^{-+} = Q^- \mathbf{A} E^+ \in B(H^+, H^-)$ ,  $\mathbf{A}^{--} = Q^- \mathbf{A} E^- \in B(H^-)$ . Also, one has

$$D = \begin{pmatrix} D^- & 0 \\ 0 & D^+ \end{pmatrix}, \quad |D| = \begin{pmatrix} -D^- & 0 \\ 0 & D^+ \end{pmatrix} \quad (3.7)$$

where  $D^\pm = \text{diag}(1/v_n)_{n \in \mathbb{Z}^\pm}$ . We get  $|D| \geq 0$  in the Hilbert space sense, i.e.,  $\langle |D| \mathbf{e}^h, \mathbf{e}^h \rangle \geq 0$  for every  $\mathbf{e}^h \in H$ .

Let  $\mathbf{e}^h = \sqrt{|D|}\mathbf{z}$ , and  $\mathbf{z} \in H$  implies  $\mathbf{e}^h \in H$ . Then the equation for  $\mathbf{z}$  is

$$\mathbf{z}_x - \mathbf{B}(x)\mathbf{z} = \mathbf{r}, \quad 0 < x < l, \quad (3.8)$$

$$\mathbf{z}^+(0) = 0, \quad \mathbf{z}^-(l) = 0, \quad (3.9)$$

where  $\mathbf{r} = (\mathbf{r}^+, \mathbf{r}^-) = \sqrt{|D|}^{-1}D\mathcal{T}^h$ , the matrix  $\mathbf{B}(x)$  is defined as  $\mathbf{B}(x) = \sqrt{|D|}^{-1}D\mathbf{A}(x)\sqrt{|D|}$ .  $\mathbf{A} \in L^1((0, l); B(H))$  implies  $\mathbf{B} \in L^1((0, l); B(H))$  since  $\sqrt{|D|} \in B(H)$ . We may write  $\mathbf{B}(x)$  in the form

$$\mathbf{B}(x) = \begin{pmatrix} -\sqrt{-D^-}\mathbf{A}^{--}(x)\sqrt{-D^-} & -\sqrt{-D^-}\mathbf{A}^{-+}(x)\sqrt{D^+} \\ \sqrt{D^+}\mathbf{A}^{+-}(x)\sqrt{-D^-} & \sqrt{D^+}\mathbf{A}^{++}(x)\sqrt{D^+} \end{pmatrix}. \quad (3.10)$$

By the norm of  $\mathbf{A}(x)$ , it is clear that

$$\|\mathbf{B}(x)\| \leq \frac{2}{\pi h} \|V\|_{L^\infty}. \quad (3.11)$$

Lemma 3.1 in [2] gave us the well-posedness for the homogeneous BVP

$$\mathbf{z}_x - \mathbf{B}(x)\mathbf{z} = 0, \quad 0 < x < l, \quad (3.12)$$

$$\mathbf{z}(0) = \mathbf{z}_0 \in H, \quad (3.13)$$

as below:

**Lemma 1** (Lemma 3.1 in [2]). *Since  $\mathbf{B} \in L^1((0, l); B(H))$ , the IVP (3.12) - (3.13) has a unique mild solution  $\mathbf{z} \in W^{1,1}((0, l); H)$ , and there exists a unique strongly continuous propagator  $U(x, x') \in B(H)$ ,  $\forall 0 \leq x, x' \leq l$ . It satisfies*

$$\frac{dU(x, 0)}{dx} - B(x)U(x, 0) = 0, \quad \frac{dU(0, x)}{dx} + U(0, x)B(x) = 0, \quad (3.14)$$

almost everywhere on  $(0, l)$ .

The propagator  $U$  in this lemma allows us to reformulate the BVP (3.8) to an IVP. Actually, the solution of the BVP (3.8) satisfies

$$\mathbf{z}(x) = U(x, 0) \begin{pmatrix} \mathbf{h}^- \\ 0 \end{pmatrix} + \int_0^x U(x, s)\mathbf{r}(s) ds = U(x, l) \begin{pmatrix} 0 \\ \mathbf{h}^+ \end{pmatrix} + \int_l^x U(x, s)\mathbf{r}(s) ds, \quad (3.15)$$

where  $\mathbf{z}^-(0) = \mathbf{h}^-$ ,  $\mathbf{z}^+(l) = \mathbf{h}^+$  are the corresponding outflow data. The idea is to calculate  $\mathbf{h}^+$  from (3.15) by eliminating  $\mathbf{h}^-$ . Noting that  $\mathbf{z}(0) = (0, \mathbf{h}^-)$  and  $\mathbf{z}(l) = (\mathbf{h}^+, 0)$ , we have the equations for  $\mathbf{h}^-$  and  $\mathbf{h}^+$

$$\begin{pmatrix} 0 \\ \mathbf{h}^+ \end{pmatrix} = U(l, 0) \begin{pmatrix} \mathbf{h}^- \\ 0 \end{pmatrix} + \int_0^l U(l, s)\mathbf{r}(s) ds, \quad (3.16)$$

$$\begin{pmatrix} \mathbf{h}^- \\ 0 \end{pmatrix} = U(0, l) \begin{pmatrix} 0 \\ \mathbf{h}^+ \end{pmatrix} + \int_l^0 U(0, s)\mathbf{r}(s) ds. \quad (3.17)$$

Applying  $P^+$  and  $P^-$  on (3.16) and (3.17) respectively yields

$$\begin{pmatrix} 0 \\ \mathbf{h}^+ \end{pmatrix} = P^+ U(l, 0) \begin{pmatrix} \mathbf{h}^- \\ 0 \end{pmatrix} + P^+ \int_0^l U(l, s) \mathbf{r}(s) ds, \quad (3.18)$$

$$\begin{pmatrix} \mathbf{h}^- \\ 0 \end{pmatrix} = P^- U(0, l) \begin{pmatrix} 0 \\ \mathbf{h}^+ \end{pmatrix} + P^- \int_l^0 U(0, s) \mathbf{r}(s) ds. \quad (3.19)$$

Eliminating  $\mathbf{h}^-$  in (3.19) and (3.18), we obtain the equation for  $\mathbf{h}^+$  as

$$(I - K) \begin{pmatrix} 0 \\ \mathbf{h}^+ \end{pmatrix} = P^+ U(l, 0) P^- \int_l^0 U(0, s) \mathbf{r}(s) ds + P^+ \int_0^l U(l, s) \mathbf{r}(s) ds, \quad (3.20)$$

where

$$K = P^+ U(l, 0) P^- U(0, l) P^+.$$

Here the operator  $K$  is the same as  $K$  defined in [2] (page 7173 Eq. (3.17)) for the homogeneous case. Making use of the skew-symmetry of  $\mathbf{A}(x)$ , it is proved in [2] that  $K$  is negative, thus  $I - K$  is invertible with a bounded inverse. We are then instantly inferred that

$$\|(I - K)^{-1}\| \leq 1.$$

As a result, it is concluded that the nonhomogeneous BVP can be transformed into an IVP, as the extension of Theorem 3.3 in [2]. Precisely, we have the following lemma:

**Lemma 2.** *The nonhomogeneous BVP (3.8) - (3.9) has a unique mild solution  $\mathbf{z} \in W^{1,1}((0, l); H)$  and*

$$\|\mathbf{z}(x)\|_{l^2} \leq 3 \exp\left(\frac{6l\|V\|_{L^\infty}}{\pi h}\right) \int_0^l \|\mathbf{r}(s)\|_{l^2} ds.$$

*Proof.* Given by [2], the self-adjointness of the bounded operator  $K$  imply that  $I - K$  is invertible with a bounded inverse, which shows the unique solvability of the BVP (3.8) - (3.9). In the following, we are going to estimate  $\|\mathbf{z}(x)\|_{l^2}$ .

In the chapter 5 of [15], it shows for every  $0 \leq x \leq x' \leq l$ ,  $U(x, x')$  is a bounded linear operator and

$$\|U(x, x')\| \leq \exp\left(\int_x^{x'} \|\mathbf{B}(s)\| ds\right),$$

thus due to (3.11),

$$\|U(x, x')\| \leq \exp\left(\frac{2|x' - x|\|V\|_{L^\infty}}{\pi h}\right) \leq \exp\left(\frac{2l\|V\|_{L^\infty}}{\pi h}\right). \quad (3.21)$$

By (3.15), we have

$$\begin{aligned} \|\mathbf{z}(x)\|_{l^2} &\leq \|U(x, l)\| \|\mathbf{h}^+\|_{l^2} + \int_0^l \|U(x, s)\| \|\mathbf{r}(s)\|_{l^2} ds \\ &\leq \|U(x, l)\| \|\mathbf{h}^+\|_{l^2} + \exp\left(\frac{2l\|V\|_{L^\infty}}{\pi h}\right) \int_0^l \|\mathbf{r}(s)\|_{l^2} ds \\ &\leq \exp\left(\frac{2l\|V\|_{L^\infty}}{\pi h}\right) \left(\|\mathbf{h}^+\|_{l^2} + \int_0^l \|\mathbf{r}(s)\|_{l^2} ds\right). \end{aligned} \quad (3.22)$$



Since  $\|(I - K)^{-1}\| \leq 1$ ,  $\|P^+\| \leq 1$ ,  $\|P^-\| \leq 1$  and by (3.21), we estimate  $\mathbf{h}^+$  using (3.20) to have

$$\|\mathbf{h}^+\|_{l^2} \leq \left( \exp\left(\frac{2l\|V\|_{L^\infty}}{\pi h}\right) + \exp\left(\frac{4l\|V\|_{L^\infty}}{\pi h}\right) \right) \int_0^l \|\mathbf{r}(s)\|_{l^2} ds. \quad (3.23)$$

Substituting (3.23) into (3.22) yields the estimate for  $\|\mathbf{z}(x)\|_{l^2}$ , i.e.,

$$\|\mathbf{z}(x)\|_{l^2} \leq 3 \exp\left(\frac{6l\|V\|_{L^\infty}}{\pi h}\right) \int_0^l \|\mathbf{r}(s)\|_{l^2} ds.$$

This ends the proof.  $\square$

Recalling the relation that  $\mathbf{e}^h = \sqrt{|D|}\mathbf{z}$ , we immediately deduce the estimate for the original BVP (3.2) - (3.3) from Lemma 2. We remark that  $\mathbf{z} \in H$  if and only if  $\mathbf{e}^h \in \tilde{H}$  where the space  $\tilde{H} = l^2(\mathbb{Z}; |v_n|)$  is a weighted  $l^2$ -space endowed with the inner product

$$(x, y)_{\tilde{H}} := \sum_{j \in J} |v_j| x_j y_j.$$

**Corollary 1.** *The BVP (3.2) - (3.3) has a unique mild solution  $\mathbf{e}^h \in W^{1,1}((0, l); \tilde{H})$ ,  $\mathbf{T} \frac{d\mathbf{e}^h}{dx} \in L^1((0, l); H)$  and*

$$\|\mathbf{e}^h\|_{\tilde{H}} \leq \frac{3}{\sqrt{\pi h}} \exp\left(\frac{6l\|V\|_{L^\infty}}{\pi h}\right) \int_0^l \|T^h(s)\|_{l^2} ds, \quad (3.24)$$

*Proof.* Noticing that  $\|\mathbf{r}(x)\|_{l^2} \leq \frac{1}{\sqrt{\pi h}} \|\mathbf{r}(x)\|_{\tilde{H}} = \frac{1}{\sqrt{\pi h}} \|T^h(x)\|_{l^2}$ , the result is inferred by Lemma 2.  $\square$

## 4 Convergence

By Corollary 1 and the triangle inequality

$$\|f^h(x, v) - f(x, v)\|_{L^2(\mathbb{R}_v)} \leq \|f^h(x, v) - t^h(x, v)\|_{L^2(\mathbb{R}_v)} + \|f(x, v) - t^h(x, v)\|_{L^2(\mathbb{R}_v)}, \quad (4.1)$$

the term  $\|f(x, v) - t^h(x, v)\|_{L^2(\mathbb{R}_v)}$  has to be estimated to have the final result on  $\|f^h(x, v) - f(x, v)\|_{L^2(\mathbb{R}_v)}$ . Obviously,  $\|f(x, v) - t^h(x, v)\|_{L^2(\mathbb{R}_v)}$  is not going to zero as  $h \rightarrow 0$  without any assumption on  $f(x, v)$ . Let us assume that  $f(x, v)$  satisfies

$$f(x, v) \in C([0, l]; L^2(\mathbb{R}_v)) \cap C^1((0, l); L^2(\mathbb{R}_v)).$$

Though this is not a rigour constraint on  $f(x, v)$ , it is enough to provide us the corresponding convergence. Since  $t^h(x, v)$  is approximating  $f(x, v)$  using the Whittaker-Shannon interpolation formula, which is a spectral expansion, a successful approximation to  $f(x, v)$  has to require a certain decay in Fourier space. With the enhanced assumption that the Fourier transformation of  $f(x, v)$  is decaying exponentially, a spectral convergence may be achieved. Precisely, from the fact that the compactly supported smooth functions  $C_c^\infty(\mathbb{R})$  are dense in  $L^2(\mathbb{R})$  and the fact that Fourier transform is a unitary transform on  $L^2(\mathbb{R})$ , the estimate of  $\|t^h - f\|_{L^1((0, l); L^2(\mathbb{R}_v))}$  is given in the following lemma.

**Lemma 3.** Let  $f(x, v) \in L^1((0, l); L^2(\mathbb{R}_v))$  and  $t^h(x, v) = \mathcal{F}_{y \rightarrow v}^{-1} \left( \widehat{f}(x, y) \zeta_h(y) \right)$  where  $\zeta_h$  is defined in (2.7), then

$$\lim_{h \rightarrow 0^+} \|f - t^h\|_{L^1((0, l); L^2(\mathbb{R}_v))} = 0.$$

Furthermore, if there exists a constant  $\alpha > 0$  such that  $\widehat{f}(x, y) \exp(\alpha|y|) \in L^1((0, l); L^2(\mathbb{R}_y))$ , then  $f^h$  converges to  $f$  with an exponential rate

$$\|f - t^h\|_{L^1((0, l); L^2(\mathbb{R}_v))} \leq C \exp\left(-\frac{\alpha}{4h}\right),$$

where  $C = \frac{1}{\sqrt{2\pi}} \|\widehat{f}(x, y) \exp(\alpha|y|)\|_{L^1((0, l); L^2(\mathbb{R}_y))}$  does not depend on  $h$ .

*Proof.* By the Parseval theorem of the Fourier transform, we have

$$\begin{aligned} \|f - t^h\|_{L^1((0, l); L^2(\mathbb{R}_v))} &= \frac{1}{\sqrt{2\pi}} \|\widehat{f} - \widehat{t^h}\|_{L^1((0, l); L^2(\mathbb{R}_y))} \\ &= \frac{1}{\sqrt{2\pi}} \int_0^l \|\widehat{f}(x, \cdot) - \widehat{f}(x, \cdot) \zeta_h(\cdot)\|_{L^2(\mathbb{R}_y)} dx. \end{aligned} \quad (4.2)$$

According to the definition of  $\zeta_h(y)$  in (2.7), we have

$$\int_0^l \|\widehat{f}(x, \cdot) - \widehat{f}(x, \cdot) \zeta_h(\cdot)\|_{L^2(\mathbb{R}_y)} dx \leq \int_0^l \left( \int_{|y| \in [\frac{R^h}{2}, \frac{3R^h}{4}]} |\widehat{f}(x, y)|^2 dy \right)^{1/2} dx. \quad (4.3)$$

It is clear the right hand side is going to zero as  $h \rightarrow 0$ . If  $\widehat{f}(x, y) \exp(\alpha|y|) \in L^1((0, l); L^2(\mathbb{R}_y))$ , obviously we have

$$\int_0^l \|\widehat{f}(x, \cdot) - \widehat{f}(x, \cdot) \zeta_h(\cdot)\|_{L^2(\mathbb{R}_y)} dx \leq \exp\left(-\frac{\alpha R^h}{2}\right) \int_0^l \left( \int_{\mathbb{R}_y} |\widehat{f}(x, y) \exp(\alpha|y|)|^2 dy \right)^{1/2} dx.$$

Noticing that  $R^h = \frac{1}{2h}$ , we finish the proof.  $\square$

In order to the estimate of  $\|e^h\|_{L^1((0, l); L^2(\mathbb{R}_v))}$  using Corollary 1, we give the estimate  $\int_0^l \|T^h(x)\|_{L^2} dx = \sqrt{2\pi h} \int_0^l \|\mathcal{T}^h(x, \cdot)\|_{L^2(\mathbb{R}_v)} dx$  in the following lemma.

**Lemma 4.** If there exists a constant  $\alpha > 0$  such that  $\frac{\partial \widehat{f}(x, y)}{\partial x} \exp(\alpha|y|) \in L^1((0, l); L^2(\mathbb{R}_y))$ , then

$$\|\mathcal{T}^h\|_{L^1((0, l); L^2(\mathbb{R}_v))} \leq Ch \exp\left(-\frac{\alpha}{4h}\right), \quad (4.4)$$

where  $C = \frac{C_\zeta}{\sqrt{2\pi}} \left\| \frac{\partial \widehat{f}(x, y)}{\partial x} \exp(\alpha|y|) \right\|_{L^1((0, l); L^2(\mathbb{R}_y))}$ .

*Proof.* By the Parseval theorem of the Fourier transform, we have

$$\|\mathcal{T}^h\|_{L^2(\mathbb{R}_v)}^2 = \frac{1}{2\pi} \|\widehat{\mathcal{T}^h}\|_{L^2(\mathbb{R}_y)}^2 = \frac{1}{2\pi} \left\| \frac{\partial}{\partial x} \widehat{f}(x, y) \zeta_h'(y) \right\|_{L^2(\mathbb{R}_y)}^2.$$

Using the properties (2.8) and (2.9) of the cutoff function, we obtain

$$\left\| \frac{\partial}{\partial x} \widehat{f}(x, y) \zeta_h'(y) \right\|_{L^2(\mathbb{R}_y)}^2 \leq C_\zeta^2 h^2 \exp\left(-\frac{\alpha R^h}{2}\right) \int_{\mathbb{R}_y} \left| \frac{\partial}{\partial x} \widehat{f}(x, y) \exp(\alpha|y|) \right|^2 dy.$$

Thus, we have

$$\|\mathcal{T}^h\|_{L^1((0,l);L^2(\mathbb{R}_v))} \leq \frac{C_\zeta h}{\sqrt{2\pi}} \exp\left(-\frac{\alpha}{4h}\right) \left\| \frac{\partial \widehat{f}(x, y)}{\partial x} \right\|_{L^1((0,l);L^2(\mathbb{R}_y))}. \quad (4.5)$$

This gives us (4.4).  $\square$

We are now ready to give the major result:

**Theorem 1.** *Let  $V(x) \in L^\infty(\mathbb{R})$ . If the continuous BVP (2.4)-(2.5) has a unique solution  $f(x, v) \in C^0([0, l]; L^2(\mathbb{R}_v)) \cap C^1((0, l); L^2(\mathbb{R}_v))$ , and there exists a constant  $\alpha > \frac{24l}{\pi} \|V\|_{L^\infty}$  such that  $\widehat{f}(x, y) \exp(\alpha|y|) \in W^{1,1}((0, l); L^2(\mathbb{R}_y))$ , then*

$$\|f^h - f\|_{L^1((0,l);L^2(\mathbb{R}_v))} \leq C \exp\left(-\frac{\beta}{h}\right),$$

where  $C = \max\left(\frac{1}{\sqrt{2\pi}}, \frac{3C_\zeta}{\sqrt{2\pi}^{3/2}}\right) \left\| \widehat{f}(x, y) \exp(\alpha|y|) \right\|_{W^{1,1}((0,l);L^2(\mathbb{R}_y))}$  and  $\beta = \frac{\alpha}{4} - \frac{6l}{\pi} \|V\|_{L^\infty}$ .

*Proof.* By Lemma 3, we have

$$\|f - t^h\|_{L^1((0,l);L^2(\mathbb{R}_v))} \leq C_1 \exp\left(-\frac{\alpha}{4h}\right), \quad (4.6)$$

where  $C = \frac{1}{\sqrt{2\pi}} \left\| \widehat{f}(x, y) \exp(\alpha|y|) \right\|_{L^1((0,l);L^2(\mathbb{R}_y))}$ .

Using the facts that

$$\|f^h(x, v) - t^h(x)\|_{L^2(\mathbb{R}_v)} = \|e^h(x, v)\|_{L^2(\mathbb{R}_v)} = \sqrt{2\pi h} \|e^h\|_{l^2},$$

$$\|\mathcal{T}^h(x, \cdot)\|_{L^2(\mathbb{R}_v)} = \sqrt{2\pi h} \|T^h(x)\|_{l^2},$$

$$\|e^h\|_{l^2} \leq \frac{1}{\sqrt{\pi h}} \|e^h\|_{\tilde{H}},$$

and by Lemma 4 and Corollary 1, we have

$$\|f^h(x, v) - t^h(x, v)\|_{L^1((0,l);L^2(\mathbb{R}_v))} \leq C_2 \exp\left(-\left(\frac{\alpha}{4} - \frac{6l}{\pi} \|V\|_{L^\infty}\right) \frac{1}{h}\right), \quad (4.7)$$

where  $C_2 = \frac{3C_\zeta}{\sqrt{2\pi}^{3/2}} \left\| \frac{\partial \widehat{f}(x, y)}{\partial x} \exp(\alpha|y|) \right\|_{L^1((0,l);L^2(\mathbb{R}_y))}$ . Then we finish the proof by (4.6), (4.7) and the triangle inequality (4.1).  $\square$

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## A Shannon Sampling Theory

We consider  $f(v)$  to be a smooth function of  $v$  in the sense its Fourier transform has a compact support, i.e.,  $\text{supp}(\hat{f}) \subset B(0, R^h)$ . According to the Shannon sampling theory (a lot of references, e.g., [8]), the function  $f(v)$  can be represented by

$$f(v) = \sum_{n=-\infty}^{\infty} f(v_n) \text{sinc} \left( R^h (v - v_n) \right), \quad (\text{A.1})$$

where  $h = \frac{1}{2R^h}$ ,  $v_n = (n+1/2)\frac{\pi}{R^h} = 2\pi(n+1/2)h$  is the  $n$ -th sampling point. The sampling frequency is higher than twice of the highest frequency of  $f$ , since  $\text{supp} \hat{f} \subset B(0, R^h)$  implies the largest  $|y|$  satisfying  $\hat{f}(y) \neq 0$  is smaller than  $R^h$ . Thus  $f(v)$  can be completely reconstructed by its values at the sampling points through (A.1). The sinc function is defined by

$$\text{sinc } x = \frac{\sin x}{x}.$$

(A.1) is then called the Whittaker-Shannon interpolation formula.

From the convolution theorem of the Fourier transform, it is easy to know that if  $f$  has a compact supported Fourier transform, i.e.  $\text{supp}(\hat{f}) \subset B(0, R^h)$ , then their convolution  $f * g(v) = \int_{\mathbb{R}} f(v - v')g(v') dv'$  has a compact supported Fourier transform

$$\mathcal{F}_{v \rightarrow y}(f * g(v)) = \hat{f}\hat{g}$$

with

$$\text{supp}(\mathcal{F}_{v \rightarrow y}(f * g(v))) \subset B(0, R^h).$$

Thus  $(f * g)(v)$  can be represented by the Whittaker-Shannon interpolation formula. Explicitly, we have the following lemma to represent  $(f * g)(v)$ .

**Lemma 5.** *Let  $f(v)$  be a function with a compactly supported Fourier transform satisfying  $\text{supp}(\hat{f}) \subset B(0, R^h)$ . Let  $g(v) \in L^2(\mathbb{R})$ . Let  $L > 2R^h$ ,  $h = \frac{1}{2R^h}$ ,  $v_n = (n + 1/2)2\pi h$  and  $\tilde{v}_n = n2\pi h$ . Then the convolution of  $f$  and  $g$  can be expressed with the Whittaker-Shannon interpolation formula (A.1),*

$$f * g(v) = \frac{2\pi}{L} \sum_{n \in \mathbb{Z}} \sum_{m \in \mathbb{Z}} g_{n-m} f_m \text{sinc} \left( \frac{L}{2}(v - v_n) \right), \quad (\text{A.2})$$

where

$$f_n = f(v_n), \quad g_n = \left( \mathcal{F}_{y \rightarrow v}^{-1} \left( \hat{g}(y) \chi_{B(0, R^h)} \right) \right) (\tilde{v}_n). \quad (\text{A.3})$$

*Proof.* By the convolution theorem of the Fourier transform, we have

$$f * g(v) = \int_{-\infty}^{\infty} f(v - v')g(v') dv' = \mathcal{F}_{y \rightarrow v}^{-1} \left( \hat{f}\hat{g} \right). \quad (\text{A.4})$$

Using  $\text{supp}(\hat{f}) \subset B(0, R^h)$ , we have

$$f * g(v) = \mathcal{F}_{y \rightarrow v}^{-1} \left( \hat{f}\hat{g} \right) = \mathcal{F}_{y \rightarrow v}^{-1} \left( \hat{f}\hat{g} \chi_{B(0, R^h)} \right) = f * \tilde{g} \quad (\text{A.5})$$

where  $\tilde{g}(v) = \mathcal{F}_{y \rightarrow v}^{-1} \left( \hat{g}(y) \chi_{B(0, R^h)(y)} \right)$ . Both  $f$  and  $\tilde{g}$  have a compactly supported Fourier transform contained in  $B(0, R^h)$  result in

$$f(v) = \sum_n f_n \operatorname{sinc} \left( R^h(v - v_n) \right), \quad \tilde{g}(v) = \sum_n g_n \operatorname{sinc} \left( R^h(v - \tilde{v}_n) \right), \quad (\text{A.6})$$

where  $g_n = \tilde{g}(\tilde{v}_n)$ . Plugging (A.6) into (A.5) and making use of using the following property (c.f. Page 13 of [8])

$$\int_{-\infty}^{\infty} \operatorname{sinc} \left( \frac{L}{2}(v - \tilde{v}_n) \right) \operatorname{sinc} \left( \frac{L}{2}(v - \tilde{v}_m) \right) dv = \frac{2\pi}{L} \delta_{nm}, \quad (\text{A.7})$$

yields (A.2). □

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