



Propagation of Gevrey regularity over long times for the fully discrete Lie Trotter splitting scheme applied to the linear Schroedinger equation

François Castella, Guillaume Dujardin

► To cite this version:

François Castella, Guillaume Dujardin. Propagation of Gevrey regularity over long times for the fully discrete Lie Trotter splitting scheme applied to the linear Schroedinger equation. *ESAIM: Mathematical Modelling and Numerical Analysis*, 2009, 43 (4), pp.651–676. 10.1051/m2an/2009028 . hal-00777098

HAL Id: hal-00777098

<https://hal.science/hal-00777098>

Submitted on 16 Jan 2013

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Propagation of Gevrey regularity over long times for the fully discrete Lie Trotter splitting scheme applied to the linear Schrödinger equation

François Castella

IRMAR & INRIA Rennes, Équipe IPSO,
Campus de Beaulieu,
Université de Rennes 1, 35042 RENNES CEDEX, FRANCE
email: `francois.castella@univ-rennes1.fr`

and

Guillaume Dujardin

INRIA Rennes, Équipe IPSO,
Antenne de Bretagne de l'École Normale Supérieure de Cachan,
Avenue Robert Schumann, 35170 BRUZ, FRANCE
email: `Guillaume.Dujardin@ens-cachan.org`

January 6, 2009

Abstract

In this paper, we study the linear Schrödinger equation over the d -dimensional torus, with small values of the perturbing potential. We consider numerical approximations of the associated solutions obtained by a symplectic splitting method (to discretize the time variable) in combination with the Fast Fourier Transform algorithm (to discretize the space variable). In this fully discrete setting, we prove that the regularity of the initial datum is preserved over long times, i.e. times that are exponentially long with the time discretization parameter. We here refer to Gevrey regularity, and our estimates turn out to be uniform in the space discretization parameter. This paper extends [6], where a similar result has been obtained in the semi-discrete situation, i.e. when the mere time variable is discretized and space is kept a continuous variable.

1 Introduction

Consider the Schrödinger equation with potential

$$\begin{cases} i\partial_t u(t, x) &= -\Delta u(t, x) + \lambda V(x)u(t, x) & (t, x) \in \mathbb{R} \times \mathbb{T}^d \\ u(0, x) &= u_0(x) & x \in \mathbb{T}^d \end{cases}$$

where u_0 is a given initial data, $V(x)$ is a real valued potential, λ is a real coupling constant that measures the strength of the potential, and \mathbb{T}^d stands for the d -dimensional torus. As is well known, the exact value $u(t, x)$ at time t is given by the propagator

$$u(t, x) = e^{-it[-\Delta + \lambda V(x)]} u_0(x).$$

It is a common idea in numerical analysis to approximate the true value of u at time t using a splitting formula, and to write

$$u(t, x) \approx \left(e^{-i\frac{t}{n}[-\Delta]} e^{-i\frac{t}{n}\lambda V(x)} \right)^n u_0(x),$$

for some large discretization parameter n . Here a Lie-Trotter splitting method has been used. Such an approximation is-called "semi-discretization" in time, in that space here has not been discretized.

In order to perform the numerical analysis of the above method, one needs at once to analyze the elementary propagator $e^{-i\frac{t}{n}[-\Delta]} e^{-i\frac{t}{n}\lambda V(x)}$, in particular in terms of propagation of u_0 's initial regularity. This is the purpose of the present paper.

For moderate values of time t , a natural framework turns out to be given by the scale of Sobolev spaces, see [2, 11]. It turns out that the splitting operator $e^{-i\frac{t}{n}[-\Delta]} e^{-i\frac{t}{n}\lambda V(x)}$ does preserve Sobolev regularity for finite values of time t , yet the estimates typically blow-up as t goes to infinity (keeping t/n small), like e^t or so. In other words, the whole analysis breaks down for large values of time in this framework.

For large values of time, the question of propagating the regularity of u_0 still is relevant, since it entails, amongst others, the conservation of energy and related invariants by the chosen numerical scheme, an important property that the original Schrödinger equation does possess. In that direction, it has been proved in [6] (see also [7] and [5]) that the building block $e^{-i\frac{t}{n}[-\Delta]} e^{-i\frac{t}{n}\lambda V(x)}$ preserves regularity of u_0 , provided λ is small enough, and V is smooth. We definitely refer here to Gevrey regularity. The need for such a smoothness, as well as for the smallness of λ , comes from two facts: firstly, we definitely wish to propagate regularity over long times t ; secondly, and in order to achieve this goal, a normal form technique is applied to obtain the desired result, a method which typically requires analyticity or Gevrey regularity, and which basically uses perturbation expansions in λ hence is only valid for small values of this parameter. Note also that such a result strongly uses the symplectic feature of the chosen splitting method, as is natural in view of the symplectic structure of the original

Schrödinger equation (see [9] for general results about the conservation of invariants by symplectic schemes, when applied to Hamiltonian Ordinary Differential Equations). This aspect somehow justifies the tools that we are here referring to.

The aim of this paper is to extend the above result of [6] (see also [7] and [5]) in the *fully discretized* case, i.e. when space is sampled as well. In practice the building block $e^{-i\frac{t}{n}[-\Delta]}$ usually is computed using the Fast Fourier Transform algorithm, while $e^{-i\frac{t}{n}\lambda V(x)}$ is a pointwise multiplication operator. We obtain estimates on the regularity of the numerical solution that do not depend on the size of the space discretization. The typical regularity of the potential function and of the unknown wave function is again of Gevrey type. To be slightly more precise, the results of this paper extend those presented in [6] in two ways: firstly, [6] only considers analytical solutions; secondly, no space discretization is made in [6] where only time discretizations are studied.

The paper is organized as follows: In Section 2, we deal with some aspects of spatial discretization of Gevrey functions. In Section 3, we prove a normal form theorem for the numerical propagator of the symplectic splitting method in the asymptotics of small potentials (Theorem 3.13). This is the core of our analysis. Next, in Section 4, we draw various consequences of our normal form theorem: in particular, we prove that the numerical solution obtained with a fully discrete, symplectic, splitting method preserves Gevrey regularity over exponentially long times (Theorem 4.10). Eventually, Section 5 is a collection of technical lemmas needed in the course of the analysis.

2 Discretisation

This section is devoted to some aspects of the discretization of Gevrey functions on a d -dimensional torus. Namely, given a smooth periodic function $V(x)$ over the torus $[-\pi; \pi]^d$, having Gevrey regularity, and given a regular sampling $(x_k)_k$ with mesh size $1/M$ where M is some (large) discretization parameter, we relate here the Gevrey smoothness of V with the properties of the discrete sampling $(V(x_k))_k$, and to that of the discrete Fourier transform $(\hat{V}_k)_k$ (see below for the precise definitions).

In the sequel, we first set up some notation that we use throughout the paper, then state and prove some approximations results, the main of whom is Lemma 2.4.

2.1 Notation

Let $d \in \mathbb{N}^*$ denote the dimension. Assume $M \in \mathbb{N}$ is given. We set

$$\mathcal{B}_M := \{k \in \mathbb{Z}^d \mid \forall i \in \{0, \dots, d\}, -M \leq k_i \leq M\}.$$

For any index $k \in \mathcal{B}_M$, we also set

$$x_k = \frac{2\pi}{2M+1}k \in [-\pi; \pi]^d.$$

$$T_k = x_k + \frac{1}{2M+1}[0, 2\pi]^d \subset [-\pi; \pi]^d$$

For any function $u \in L^1(\mathbb{T}^d)$, we define the Fourier transform

$$\forall k \in \mathbb{Z}^d, \quad \hat{u}_k = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} u(x) e^{-ikx} dx,$$

where kx stands for the scalar product of the two vectors, without further specification. For any $z = (z_1, \dots, z_d) \in \mathbb{C}^d$, we denote

$$|z| = \sqrt{|z_1|^2 + \dots + |z_d|^2} \quad \text{and} \quad |z|_\infty = \max\{|z_1|, \dots, |z_d|\}.$$

Throughout the paper, bold letters denote linear operators on $\mathbb{C}^{(2M+1)^d}$ or vectors of $\mathbb{C}^{(2M+1)^d}$ whose norms (to be defined later) are to be estimated by bounds that do not depend on M . When typing bold letters, we use upper case letters for linear operators and lower case letters for vectors.

Finally, for all $M \in \mathbb{N}$, we denote by $\mathbf{W} = [\mathbf{W}_{k,\ell}]_{(k,\ell) \in \mathcal{B}_M \times \mathcal{B}_M}$ the linear operator, or matrix, associated with the discrete Fourier transform, through the coefficients

$$\mathbf{W}_{k,\ell} = \frac{1}{(2M+1)^{d/2}} e^{-ikx_\ell}, \quad \text{whenever } k, \ell \in \mathcal{B}_M.$$

The operator \mathbf{W} naturally is unitary,

$$(\mathbf{W}^*)\mathbf{W} = \text{Id}_{(2M+1)^d}. \quad (2.1)$$

2.2 Approximation results

Assume V is a complex function on \mathbb{T}^d . Denoting

$$\forall k, \ell \in \mathcal{B}_M, \quad \mathbf{V}_{k,\ell} = \begin{cases} 0 & \text{if } k \neq \ell \\ V(x_k) & \text{if } k = \ell \end{cases},$$

the operator \mathbf{V} collects the sampled values of V at the discretization points x_k , and \mathbf{V} somehow provides an approximation of the original V to within $\mathcal{O}(1/M)$, provided V has $W^{1,\infty}$ smoothness, say.

The discrete Fourier transform of the sampled values \mathbf{V} is provided by the coefficients

$$(\mathbf{WVW}^*)_{k,\ell} = \frac{1}{(2M+1)^d} \sum_{p \in \mathcal{B}_M} V(x_p) e^{-i(k-\ell)x_p}, \quad \text{whenever } k, \ell \in \mathcal{B}_M.$$

Note that for all $j \in \{1, \dots, d\}$, $\left| \partial_{x_j} (e^{-i(k-\ell)x} V(x)) \right| \leq (1+|k-\ell|) \|V\|_{W^{1,\infty}}$. This fact ensures that the coefficients of \mathbf{WVW}^* approximate the Fourier transform \hat{V} to within $\mathcal{O}(1/M)$, in the following sense:

Lemma 2.1 *For all $V \in W^{1,\infty}$, we have*

$$\forall M \in \mathbb{N}, \forall k \in \mathcal{B}_M, \quad \left| \hat{V}_{k-\ell} - (\mathbf{WVW}^*)_{k,\ell} \right| \leq \frac{2\pi \|V\|_{W^{1,\infty}}}{2M+1} (1 + |k-\ell|). \quad (2.2)$$

Obviously, the convergence rate $1/M$ in the above Lemma is optimal, even for very smooth V 's. However, the linear growth with $|k-\ell|$ of the above error term is to be improved as the smoothness of V becomes higher. This is the question we now investigate, in the case when V has Gevrey smoothness.

Our main result in this direction is Lemma 2.4 below.

Definition 2.2 *A complex function $V \in L^1(\mathbb{T}^d)$ is said to be (ρ_V, α) -Gevrey for some $\rho_V > 0$ and $\alpha \geq 1$ if there exists $\delta > 0$ such that for all $k \in \mathbb{Z}^d$, $|\hat{V}_k| \leq M_V e^{-(\rho_V + \delta)|k|^{1/\alpha}}$.*

Definition 2.3 *For all (ρ_V, α) -Gevrey function on \mathbb{T}^d , we define the corresponding norm by setting*

$$\|V\|_{\rho_V, \alpha} = \sup_{p \in \mathbb{Z}^d} |\hat{V}_p| e^{\rho_V |p|^{1/\alpha}}.$$

Lemma 2.4 *Assume V is a (ρ_V, α) -Gevrey function. Then, there exists a positive constant $M_V^{(1)}$ depending on V and d such that*

$$\forall M \in \mathbb{N}, \forall (k, \ell) \in \mathcal{B}_M, \quad \left| \hat{V}_{k-\ell} - (\mathbf{WVW}^*)_{k,\ell} \right| \leq \frac{2\pi M_V^{(1)}}{2M+1} e^{-\rho_V |k-\ell|^{1/\alpha}}.$$

Proof. For $k, \ell \in \mathcal{B}_M$, we write

$$\frac{1}{(2M+1)^d} V(x_p) e^{-i(k-\ell)x_p} = \frac{1}{(2\pi)^d} \int_{T_p} V(x_p) e^{-i(k-\ell)x_p} dx.$$

Hence, using the additivity of the integral in the definition of $\hat{V}_{k,\ell}$, we get

$$(\mathbf{WVW}^*)_{k,\ell} - \hat{V}_{k-\ell} = \frac{1}{(2\pi)^d} \sum_{p \in \mathcal{B}_M} \int_{T_p} (V(x_p) e^{-i(k-\ell)x_p} - V(x) e^{-i(k-\ell)x}) dx.$$

Set for all $x \in \mathbb{T}^d$,

$$f_{k,\ell}(x) := V(x) e^{-i(k-\ell)x}$$

and note that

$$\nabla f_{k,\ell}(x) = (\nabla V(x) - i(k-\ell)V(x)) e^{-i(k-\ell)x} =: g_{k-\ell}(x) e^{-i(k-\ell)x},$$

up to defining the auxiliary function

$$g_{k-\ell}(x) := \nabla V(x) - i(k-\ell)V(x).$$

Since

$$f(x_p) - f(x) = (x_p - x) \int_0^1 \nabla f_{k,\ell}(tx_p + (1-t)x) dt,$$

we recover,

$$\begin{aligned} (\mathbf{WVW}^*)_{k,\ell} - \hat{V}_{k-\ell} &= (2\pi)^{-d} \sum_{p \in \mathcal{B}_M} \int_{T_p} (x_p - x) \left(\int_0^1 \nabla f_{k,\ell}(tx_p + (1-t)x) dt \right) dx \\ &= -(2\pi)^{-d} \sum_{p \in \mathcal{B}_M} \int_{T_0} \int_0^1 u g_{k-\ell}(x_p + (1-t)u) e^{i(k-\ell)(x_p + (1-t)u)} dt du. \end{aligned}$$

Now, it turns out that the discrete Fourier inversion formula provides, for any $z \in \mathbb{R}^d$, the identity

$$\sum_{p \in \mathcal{B}_M} g_{k-\ell}(x_p + z) e^{i(k-\ell)(x_p + z)} = (2M+1)^d (\hat{g}_{k-\ell})_{k-\ell}.$$

Therefore we recover

$$(\mathbf{WVW}^*)_{k,\ell} - \hat{V}_{k-\ell} = -(2\pi)^{-d} (2M+1)^d (\hat{g}_{k-\ell})_{k-\ell} \int_{T_0} u du,$$

which implies, using that the measure of T_0 is $(\frac{2\pi}{2M+1})^d$,

$$\left| (\mathbf{WVW}^*)_{k,\ell} - \hat{V}_{k-\ell} \right| \leq \frac{2\pi\sqrt{d}}{2M+1} |(\hat{g}_{k-\ell})_{k-\ell}|.$$

To conclude the proof, note that, since V is (ρ_V, α) -Gevrey, we have for some $M, \delta > 0$ and all $j \in \{1, \dots, d\}$,

$$\begin{aligned} |(\hat{g}_{k-\ell})_{k-\ell}| &\leq 2|k-\ell| |\hat{V}_{k-\ell}| \\ &\leq M|k-\ell| e^{-(\rho_V + \delta)|k-\ell|^{1/\alpha}} \\ &\leq C_\delta M e^{-\rho_V |k-\ell|^{1/\alpha}}, \end{aligned}$$

with $C_\delta = \sup_{p \in \mathbb{Z}^d} |p| e^{-\delta|p|^{1/\alpha}}$. ■

As an immediate consequence of the above Lemma, we deduce that the operator \mathbf{WVW}^* is (ρ_V, α) -Gevrey for all M , with a norm independant of M , in the following sense:

Definition 2.5 Set $M \in \mathbb{N}$, $\rho > 0$, $\alpha \geq 1$. For all operator $\mathbf{A} = (\mathbf{A}_{k,\ell})_{k,\ell \in \mathcal{B}_M} \in \mathbb{C}^{(2M+1)^{2d}}$, we define the (ρ, α) -Gevrey norm by setting

$$\|\mathbf{A}\|_{\rho,\alpha} = \sup_{k,\ell \in \mathcal{B}_M} |\mathbf{A}_{k,\ell}| e^{\rho|k-\ell|^{1/\alpha}}.$$

Corollary 2.6 Assume V is a (ρ_V, α) -Gevrey function. Then, there exists a positive constant $M_V^{(2)}$ such that

$$\forall M \in \mathbb{N}, \quad \|\mathbf{WVW}^*\|_{\rho_V, \alpha} \leq M_V^{(2)}.$$

Proof. Use the regularity of V provided by Definition 2.2 and the result of Lemma 2.4 to conclude by the triangle inequality. ■

Lemma 2.7 Assume \mathbf{A} and \mathbf{B} are (sequences of) operators such that there exist $\mathcal{A}, \mathcal{B} > 0$ such that

$$\forall M \in \mathbb{N} \quad \|\mathbf{A}\|_{\rho, \alpha} \leq \mathcal{A} \quad \text{and} \quad \|\mathbf{B}\|_{\rho+\delta, \alpha} \leq \mathcal{B},$$

for some $\rho, \delta > 0$ and $\alpha \geq 1$. Then there exists a constant $C > 1$ depending only on α and δ such that

$$\forall M \in \mathbb{N}, \quad \|\mathbf{AB}\|_{\rho, \alpha} \leq C\mathcal{A}\mathcal{B}.$$

Remark 2.8 Lemma 2.7 provides sufficient conditions on (sequences of) operators \mathbf{A} and \mathbf{B} to control the norm of the product \mathbf{AB} independently of M .

Note that our proof establishes the above constant C does not depend on $M, \mathbf{A}, \mathbf{B}$, nor on \mathcal{A} and \mathcal{B} . It may be chosen as

$$C = \sum_{p \in \mathbb{Z}^d} e^{-\delta|p|^{1/\alpha}}.$$

Proof. Since $\alpha \geq 1$, we have for all $x, y \in \mathbb{R}^d$,

$$\begin{aligned} |x - y|^{1/\alpha} &\leq (|x| + |y|)^{1/\alpha} \\ &\leq |x|^{1/\alpha} + |y|^{1/\alpha}. \end{aligned}$$

Hence, for all $M \in \mathbb{N}$ and all $k, \ell \in \mathcal{B}_M$,

$$\begin{aligned} |\mathbf{AB}_{k, \ell}| e^{\rho|k-\ell|^{1/\alpha}} &\leq \mathcal{A}\mathcal{B} \sum_{p \in \mathcal{B}_M} e^{-\rho(|k-p|^{1/\alpha} + |p-\ell|^{1/\alpha} - |k-\ell|^{1/\alpha})} e^{-\delta|p-\ell|^{1/\alpha}} \\ &\leq \mathcal{A}\mathcal{B} \sum_{p \in \mathbb{Z}^d} e^{-\delta|p-\ell|^{1/\alpha}}. \end{aligned}$$

The conclusion follows. ■

Corollary 2.9 Assume V is a (ρ_V, α) -Gevrey function. Then, there exists a positive constant $M_V^{(3)}$ such that

$$\forall M \in \mathbb{N}, \forall n \in \mathbb{N}^*, \quad \|(\mathbf{WVW}^*)^n\|_{\rho_V, \alpha} \leq (M_V^{(3)})^n. \quad (2.3)$$

Remark 2.10 Note that, thanks to the unitarity of \mathbf{W} , we have $(\mathbf{WVW}^*)^n = \mathbf{WV}^n \mathbf{W}^*$.

Proof. Use the Definition 2.2 and adapt Corollary 2.6 to get a constant $M_0 > 0$ such that for some $\delta > 0$, for all $M \in \mathbb{N}$,

$$\|\mathbf{WVW}^*\|_{\rho_V + \delta, \alpha} \leq M_0.$$

The previous corollary yields for all $n \in \mathbb{N}$ and all $M \in \mathbb{N}^*$,

$$\|\mathbf{WV}^{n+1} \mathbf{W}^*\|_{\rho_V, \alpha} \leq C M_V^{(3)} \|\mathbf{WV}^n \mathbf{W}^*\|_{\rho_V, \alpha},$$

and the result follows by induction. ■

3 A normal form theorem

This section is devoted to the statement and proof of a normal form theorem for the fully discrete symplectic splitting propagator that we discussed informally in the introduction. This technical statement lies at the core of our analysis. Our main Theorem in this section is Theorem 3.13. Note that the techniques and the method of proof that we use here is directly inspired from [6] (see also [7] and [5]).

In the remainder part of the present article, we make the

Hypothesis 3.1 *V is a complex (ρ_V, α) -Gevrey function for some $\rho_V > 0$ and $\alpha \geq 1$.*

This section is organized as follows: we first set up some notation, including the definition of the numerical propagator that we consider. We then seek a normal form for the propagator, using power series expansions in the parameter λ . Expanding the natural identity that lies at the core of our normal form approach, it turns out, as usual, that we need to iteratively solve a homological equation (Equation (3.5)). This is done using a non-resonance assumption on the time step, namely Hypothesis 3.2. With the help of this assumption, we then prove estimates for the coefficients of the power series involved in the normal form theorem (Proposition 3.9 and Lemma 3.10). Eventually, summing up the various estimates in the appropriate way, we state and prove the normal form theorem (Theorem 3.13).

3.1 Notation

For $M \in \mathbb{N}$, we denote by Δ the collection of coefficients defined by

$$\forall k, \ell \in \mathcal{B}_M, \quad \Delta_{k, \ell} = \begin{cases} 0 & \text{if } k \neq \ell \\ -|k|^2 & \text{if } k = \ell \end{cases}.$$

Note that Δ is a spectral approximation of the Laplacian operator on the d -dimensional torus \mathbb{T}^d .

For $\lambda \in \mathbb{R}$ and $h > 0$, we denote

$$\mathbf{L}(\lambda) = e^{ih\Delta} \mathbf{W} e^{-ih\lambda \mathbf{V}} \mathbf{W}^* = e^{ih\Delta} e^{-ih\lambda \mathbf{W} \mathbf{V} \mathbf{W}^*}. \quad (3.1)$$

We consider the operator $\mathbf{L}(\lambda)$ as the numerical approximation of the exact propagator associated with the linear Schrödinger equation

$$\begin{cases} i\partial_t u(t, x) &= -\Delta u(t, x) + \lambda V(x)u(t, x) & (t, x) \in \mathbb{R} \times \mathbb{T}^d \\ u(0, x) &= u_0(x) & x \in \mathbb{T}^d \end{cases}, \quad (3.2)$$

where u_0 is a given complex function on \mathbb{T}^d . As explained in the introduction, operator $\mathbf{L}(\lambda)$ is obtained by using a Lie-Trotter splitting method (to discretize

the time variable), in combination with the Fast Fourier Transform algorithm (to discretize space). In other words, the operator $\mathbf{L}(\lambda)$ coincides, in practice, with

$$\mathbf{L}(\lambda) \sim e^{ih\Delta} \text{FFT} e^{-ih\lambda V(x)} \text{FFT}^{-1}.$$

In these variables, the time step h obviously plays the role of the t/n in the introduction.

3.2 Seeking a normal form for \mathbf{L}

Recall that our goal is to prove that operator $\mathbf{L}(\lambda)$ propagates Gevrey regularity over long times. As in [6] (see also [7] and [5]), our strategy is to deduce propagation of smoothness from a (stronger) normal form result. In that respect, we readily seek formal operator series expansions $\mathbf{Q} = \mathbf{Q}(\lambda) = \sum_n \lambda^n \mathbf{Q}_n$ and $\Sigma = \Sigma(\lambda) = \sum_n \lambda^n \Sigma_n$, which are L_2 -unitary, and such that

$$\mathbf{Q}(\lambda) \mathbf{L}(\lambda) \mathbf{Q}(\lambda)^* = \Sigma(\lambda). \quad (3.3)$$

In other words, we wish to conjugate $\mathbf{L}(\lambda)$ with a unitary matrix $\Sigma(\lambda)$, which hopefully has a "simple form". Note that the particular value $\lambda = 0$ readily provides

$$\mathbf{Q}_0 e^{ih\Delta} \mathbf{Q}_0^* = \Sigma_0,$$

which somehow leads to the natural (yet arbitrary) choice

$$\mathbf{Q}_0 = \text{Id}_{(2M+1)^d}, \quad \Sigma_0 = e^{ih\Delta}.$$

In other words, $\mathbf{Q}(\lambda)$ will be constructed as a λ -perturbation of the identity, while $\Sigma(\lambda)$ appears as a λ -perturbation of the free propagator $e^{ih\Delta}$.

Now, as in [6], to compute the higher order terms \mathbf{Q}_n, Σ_n , whenever $n \geq 1$, we use the following trick: since unitarity involves a nonlinear condition (a matrix \mathbf{U} is unitary whenever the quadratic condition $\mathbf{U} \mathbf{U}^* = \text{Id}$ is met), instead of seeking $\mathbf{Q}(\lambda)$ and $\Sigma(\lambda)$, we rather argue on the logarithm of these matrices. The latter indeed should be hermitian matrices, which involves a simpler, linear condition ($\mathbf{H}^* = \mathbf{H}$). Technically speaking, we shall actually argue on the logarithmic derivatives of these matrices with respect to λ . For this reason, we now introduce $\mathbf{S}(\lambda)$ and $\mathbf{X}(\lambda)$ defined by

$$\begin{aligned} \mathbf{S}(\lambda) &= i \mathbf{Q}^*(\lambda) \partial_\lambda \mathbf{Q}(\lambda), \\ \mathbf{X}(\lambda) &= i \Sigma^*(\lambda) \partial_\lambda \Sigma(\lambda), \end{aligned}$$

and look for the value of $\mathbf{S}(\lambda)$ and $\mathbf{X}(\lambda)$ rather than that of $\mathbf{Q}(\lambda)$ and $\Sigma(\lambda)$. Naturally, the value of $\mathbf{Q}(\lambda)$ and $\Sigma(\lambda)$ is easily reconstructed from $\mathbf{S}(\lambda)$ and $\mathbf{X}(\lambda)$ using the differential equalities $i \partial_\lambda \mathbf{Q}(\lambda) = \mathbf{Q}(\lambda) \mathbf{S}(\lambda)$ and $i \partial_\lambda \Sigma(\lambda) = \Sigma(\lambda) \mathbf{X}(\lambda)$, together with the initial values $\mathbf{Q}(0) = \text{Id}_{(2M+1)^d}$, $\Sigma(0) = e^{ih\Delta}$.

Differentiating relation (3.3) with respect to λ , using the relations

$$\mathbf{S}(\lambda) = i \mathbf{Q}^*(\lambda) \partial_\lambda \mathbf{Q}(\lambda) = -i (\partial_\lambda \mathbf{Q}(\lambda))^* \mathbf{Q}(\lambda),$$

(since $\mathbf{S}(\lambda)$ is hermitian) and similarly for $\mathbf{X}(\lambda)$ to remove all terms $\partial_\lambda \mathbf{Q}(\lambda)$ and $\partial_\lambda \mathbf{\Sigma}(\lambda)$, next using again the relation $\mathbf{\Sigma}(\lambda) = \mathbf{Q}(\lambda) \mathbf{L}(\lambda) \mathbf{Q}^*(\lambda)$, and lastly using the unitarity of $\mathbf{Q}(\lambda)$, $\mathbf{L}(\lambda)$ to factorize and eventually eliminate these terms whenever possible, establishes that $\mathbf{X}(\lambda)$ and $\mathbf{S}(\lambda)$ should satisfy

$$\mathbf{S}(\lambda) - \mathbf{L}^*(\lambda) \mathbf{S}(\lambda) \mathbf{L}(\lambda) = h \mathbf{W} \mathbf{V} \mathbf{W}^* - \mathbf{Q}^*(\lambda) \mathbf{X}(\lambda) \mathbf{Q}(\lambda). \quad (3.4)$$

Here it is intended that $\mathbf{S}(\lambda) = \sum_n \lambda^n \mathbf{S}_n$ and $\mathbf{X}(\lambda) = \sum_n \lambda^n \mathbf{X}_n$ are sums of hermitian operators. We now solve equation (3.4) in the unknowns $\mathbf{S}(\lambda)$, $\mathbf{X}(\lambda)$ using a perturbation procedure, recalling that $\mathbf{Q}(\lambda)$ is related to $\mathbf{S}(\lambda)$ through $i \partial_\lambda \mathbf{Q}(\lambda) = \mathbf{Q}(\lambda) \mathbf{S}(\lambda)$.

Expanding relation (3.4) in powers of λ and equating like powers provides the necessary relation

$$\begin{aligned} \mathbf{S}_n - \sum_{p+q+r=n} \frac{(ih \mathbf{W} \mathbf{V} \mathbf{W}^*)^p}{p!} e^{-ih\Delta} \mathbf{S}_q e^{ih\Delta} \frac{(-ih \mathbf{W} \mathbf{V} \mathbf{W}^*)^r}{r!} \\ = h \mathbf{W} \mathbf{V} \mathbf{W}^* \mathbf{1}_{n=0} - \sum_{p+q+r=n} \mathbf{Q}_p^* \mathbf{X}_q \mathbf{Q}_r, \end{aligned}$$

which also reads

$$\begin{aligned} \mathbf{S}_n - e^{-ih\Delta} \mathbf{S}_n e^{ih\Delta} + \mathbf{X}_n = h \mathbf{W} \mathbf{V} \mathbf{W}^* \mathbf{1}_{n=0} \\ + \sum_{\{p+q+r=n | q \neq n\}} \left(\mathbf{W} \frac{(ih \mathbf{V})^p}{p!} \mathbf{W}^* e^{-ih\Delta} \mathbf{S}_q e^{ih\Delta} \mathbf{W} \frac{(-ih \mathbf{V})^r}{r!} \mathbf{W}^* - \mathbf{Q}_p^* \mathbf{X}_q \mathbf{Q}_r \right). \end{aligned} \quad (3.5)$$

This is the homological equation that we now aim at solving. In principle, equation 3.5 should enable us to compute \mathbf{S}_{n+1} , \mathbf{X}_{n+1} , \mathbf{Q}_{n+1} from \mathbf{S}_n , \mathbf{X}_n , \mathbf{Q}_n , by iteratively inverting the operator $\mathbf{S} \mapsto \mathbf{S} - e^{-ih\Delta} \mathbf{S} e^{ih\Delta}$. For that reason, and due to possible resonances in this operators (particular values of h that make the kernel of $\mathbf{S} \mapsto \mathbf{S} - e^{-ih\Delta} \mathbf{S} e^{ih\Delta}$ degenerate), it is readily clear that the homological equation can have no solution or infinitely many solutions, depending on the value of h .

3.3 Solving the homological equation (3.5)

In order to be able to solve equation (3.5), and more importantly to derive estimates for its solutions, we use the following

Hypothesis 3.2 *There exists $\gamma > 0$ and $\nu > 1$ such that*

$$\forall k \in \mathbb{Z}, \quad k \neq 0, \quad \left| \frac{1 - e^{ikh}}{h} \right| \geq \frac{\gamma}{|k|^\nu}. \quad (3.6)$$

Hypothesis 3.2 obviously is a non-resonance condition on $h > 0$. As it becomes clear later, it will be used to ensure, amongst others, that the kernel of the mapping $\mathbf{S} \mapsto \mathbf{S} - e^{-ih\Delta}\mathbf{S}e^{ih\Delta}$ is indeed "non-degenerate", and that its inverse is "reasonably bounded".

It is worth noticing that Hypothesis 3.2 is generically satisfied, see [9]. Hence Hypothesis 3.2 is essentially harmless.

Definition 3.3 For $K > 0$, we define

$$I_K = \{(k, \ell) \in \mathcal{B}_M \times \mathcal{B}_M \mid (|k| \leq K \text{ or } |\ell| \leq K)\}.$$

For $h > 0$ satisfying (3.6), we define the I_K -solution of the equation

$$\mathbf{S} - e^{ih\Delta}\mathbf{S}e^{-ih\Delta} + \mathbf{X} = \mathbf{G}, \quad (3.7)$$

where G is a given hermitian operator on $\mathbb{C}^{(2M+1)^d}$, as the couple (\mathbf{S}, \mathbf{X}) of hermitian operators on $\mathbb{C}^{(2M+1)^d}$, defined by their coefficients $\mathbf{S}_{k,\ell}$ and $\mathbf{X}_{k,\ell}$ ($k, \ell \in \mathcal{B}_M$) through

$$\mathbf{S}_{k,\ell} = \begin{cases} 0 & \text{if } |k| = |\ell| \text{ or } (k, \ell) \notin I_K \\ (1 - e^{-ih(|k|^2 - |\ell|^2)})^{-1} \mathbf{G}_{k,\ell} & \text{otherwise} \end{cases},$$

and

$$\mathbf{X}_{k,\ell} = \begin{cases} -\mathbf{G}_{k,\ell} & \text{if } |k| = |\ell| \text{ or } (k, \ell) \notin I_K \\ 0 & \text{otherwise} \end{cases}.$$

Remark 3.4 The above definition is motivated by the following observation. The mapping $\mathbf{S} \mapsto \mathbf{S} - e^{-ih\Delta}\mathbf{S}e^{ih\Delta}$ coincides, in coordinates, with the diagonal operator $\mathbf{S}_{k,\ell} \mapsto (1 - e^{-ih(|k|^2 - |\ell|^2)})\mathbf{S}_{k,\ell}$. Hence inverting the above operator requires to deal with the possibly singular factors $(1 - e^{-ih(|k|^2 - |\ell|^2)})^{-1}$. Whenever $|k|^2 = |\ell|^2$, the denominator vanishes and the choice $\mathbf{X}_{k,\ell} = -\mathbf{G}_{k,\ell}$ is actually necessary in this case. On the other hand, when $|k|^2 \neq |\ell|^2$, the factor $(1 - e^{-ih(|k|^2 - |\ell|^2)})^{-1}$ is well-defined (since h is non-resonant). However, the non-resonance condition only ensures that $(1 - e^{-ih(|k|^2 - |\ell|^2)})^{-1}$ has size $\frac{\gamma}{h} \mathcal{O}([|k|^2 - |\ell|^2]^\nu) = \frac{\gamma}{h} \mathcal{O}(|k - \ell|^\nu |k + \ell|^\nu)$, an estimate which degenerates into $\frac{\gamma K^\nu}{h} \mathcal{O}(|k - \ell|^\nu)$ whenever $(k, \ell) \in I_K$, a diverging estimate as K grows. This explains the role of our truncation parameter K , which cuts off large frequencies, and our definition of \mathbf{X} eventually gathers all contributions that are related with possible divergences of the factors $(1 - e^{-ih(|k|^2 - |\ell|^2)})^{-1}$.

All these considerations justify the following

Definition 3.5 A linear operator \mathbf{X} on $\mathbb{C}^{(2M+1)^d}$ satisfying

$$\forall (k, \ell) \in \mathcal{B}_M^2, \quad \left(\mathbf{X}_{k,\ell} \neq 0 \Rightarrow (|k| = |\ell| \text{ or } (k, \ell) \notin I_K) \right)$$

is said to be K -almost- X -shaped, or simply almost- X -shaped.

Remark 3.6 Note that the name comes from the usual matrix notation when $d = 1$.

We have the following estimates for the solutions of Equation (3.5):

Proposition 3.7 For all $\rho > 0$, $\delta \in (0, \rho)$, $\alpha \geq 1$, $K \geq 1$, and all operator \mathbf{G} , the I_K -solution (\mathbf{X}, \mathbf{S}) of Equation (3.7) satisfies

$$\|\mathbf{X}\|_{\rho, \alpha} \leq \|\mathbf{G}\|_{\rho, \alpha} \quad \text{and} \quad \|\mathbf{S}\|_{\rho - \delta, \alpha} \leq \left(\frac{2\nu\alpha}{\delta}\right)^{2\nu\alpha} \frac{2^{2\nu} K^\nu}{\gamma h} \|\mathbf{G}\|_{\rho, \alpha}.$$

Remark 3.8 Needless to say, the estimates of Proposition 3.7 will be used repeatedly in the sequel, to solve equation (3.5) and to sum up the associated series expansion $\sum_n \lambda^n \mathbf{S}_n$ and $\sum_n \lambda^n \mathbf{X}_n$.

Proof. The fact that $\|\mathbf{X}\|_{\rho, \alpha} \leq \|\mathbf{G}\|_{\rho, \alpha}$ is obvious from the definition of I_K -solutions.

Now, to estimate \mathbf{S} , the difficulty is to replace $k \in \mathbb{Z}$ in Hypothesis (3.6) by $|k|^2 - |\ell|^2$ whenever $(k, \ell) \in I_K$. To do so, we write for $(k, \ell) \in I_K$

$$\begin{aligned} ||k|^2 - |\ell|^2|^2 &= |k - \ell| |k + \ell| \leq |k - \ell| (|k - \ell| + 2K) \\ &\quad (\text{since } (k, \ell) \in I_K) \\ &= |k - \ell|^2 + 2K|k - \ell| \leq |k - \ell|^2 + 2K|k - \ell|^2 \\ &\quad (\text{here we used the fact that } |k - \ell| \text{ is either } = 0, \text{ or it is } \geq 1) \\ &\leq 4K|k - \ell|^2. \end{aligned}$$

Therefore, for $(k, \ell) \in I_K$, with $|k| \neq |\ell|$, we derive using Hypothesis 3.2 the estimate

$$\begin{aligned} |\mathbf{S}_{k, \ell}| e^{(\rho - \delta)|k - \ell|^{1/\alpha}} &\leq |(1 - e^{-ih(|k|^2 - |\ell|^2)})^{-1}| |\mathbf{G}_{k, \ell}| e^{(\rho - \delta)|k - \ell|^{1/\alpha}} \\ &\leq \frac{\|\mathbf{G}\|_{\rho, \alpha}}{\gamma h} ||k|^2 - |\ell|^2|^\nu e^{-\rho|k - \ell|^{1/\alpha}} e^{(\rho - \delta)|k - \ell|^{1/\alpha}} \\ &\leq \|\mathbf{G}\|_{\rho, \alpha} \frac{2^{2\nu} K^\nu}{\gamma h} |k - \ell|^{2\nu} e^{-\delta|k - \ell|^{1/\alpha}}. \end{aligned}$$

The fact that

$$\forall x \geq 0, \quad x^{2\nu} e^{-\delta x^{1/\alpha}} \leq \left(\frac{2\nu\alpha}{\delta}\right)^{2\nu\alpha} e^{-2\nu\alpha}$$

implies the result. ■

3.4 Estimates for the coefficients

3.4.1 Estimates for \mathbf{S} and \mathbf{X}

Proposition 3.9 There exist constants $C_0 \geq 1$ and $K_0 \geq 1$ depending only on V , $M_V^{(3)}$, ρ_V , α , γ , ν and d such that for all $K \geq K_0$ and all $h \in (0, 1)$

satisfying (3.6), we have the following estimates for the iterative I_K -solutions of the homological equation (3.5):

for all $J \geq 1$ and all $M \in \mathbb{N}$, we have

$$\|\mathbf{S}_J\|_{\rho_V/3,\alpha} + \|\mathbf{Q}_J\|_{\rho_V/3,\alpha} \leq (C_0 K^{\mu_1} J^{\mu_2})^J \quad \text{and} \quad (3.8)$$

$$\|\mathbf{X}_J\|_{\rho_V/3,\alpha} \leq h (C_0 K^{\mu_1} J^{\mu_2})^J, \quad (3.9)$$

where $\mu_1 = 2\nu$ and $\mu_2 = 3\alpha d + 3 + 4\nu\alpha$.

Proof. Let $J \geq 1$ be a fixed integer. We set

$$\delta = \frac{\rho_V}{(2J+1)}.$$

Besides, for $j \in \{0, \dots, J+1\}$, we also define

$$\rho_j = \rho_V - j\delta = (2J+1-j)\delta.$$

In the sequel, for all operator \mathbf{A} and for $j \in \{0, \dots, J+1\}$, we set

$$\|\mathbf{A}\|_{(j)} := \|\mathbf{A}\|_{\rho_j,\alpha}.$$

Note that if $0 \leq j \leq k \leq J+1$, then $\|\mathbf{A}\|_{(k)} \leq \|\mathbf{A}\|_{(j)}$. Moreover, $\|\mathbf{A}\|_{(0)} = \|\mathbf{A}\|_{\rho_V,\alpha}$ and $\|\mathbf{A}\|_{(J+1)} = \|\mathbf{A}\|_{\rho_V J/(2J+1),\alpha} \geq \|\mathbf{A}\|_{\rho_V/3,\alpha}$.

Let us now come to estimating \mathbf{S}_j , \mathbf{X}_j , \mathbf{Q}_j provided by the homological equation and relation $i\partial_\lambda \mathbf{Q}(\lambda) = \mathbf{Q}(\lambda)\mathbf{S}(\lambda)$, whenever $j \geq 0$. The proof is in two steps.

First step.

For $j = 0$, using Corollary 2.6, Proposition 3.7, and the fact that $\mathbf{Q}_0 = \text{Id}_{(2M+1)^d}$, readily provides

$$\|\mathbf{S}_0\|_{(1)} \leq M_V^{(3)} \left(\frac{2\nu\alpha}{\delta} \right)^{2\nu\alpha} \frac{2^{2\nu} K^\nu}{\gamma h}, \quad \|\mathbf{X}_0\|_{(0)} \leq h M_V^{(3)} \quad \text{and} \quad \|\mathbf{Q}_0\|_{(0)} = 1.$$

For later values of j , using once again the relation $i\partial_\lambda \mathbf{Q}(\lambda) = \mathbf{Q}(\lambda)\mathbf{S}(\lambda)$, and expanding in powers of λ provides the following identity

$$i(j+1)\mathbf{Q}_{j+1} = \sum_{k=0}^j \mathbf{Q}_k \mathbf{S}_{j-k}.$$

It implies, together with Lemma 2.7, that

$$(j+1)\|\mathbf{Q}_{j+1}\|_{(j+1)} \leq \sum_{k=0}^j \|\mathbf{Q}_k \mathbf{S}_{j-k}\|_{(j+1)} \leq \tilde{C} \sum_{k=0}^j \|\mathbf{Q}_k\|_{(j)} \|\mathbf{S}_{j-k}\|_{(j+1)}.$$

Note that the constant \tilde{C} depends on α and δ , and hence on J . We may actually take (see Lemma 2.7).

$$\tilde{C} = \sum_{p \in \mathbb{Z}^d} e^{-\delta|p|^{1/\alpha}}.$$

By Corollary 5.3, whose proof is postponed as well, it turns out there exists a constant $C_{\alpha,d,\rho_V} > 0$ such that

$$\tilde{C} \leq \frac{C_{\alpha,d,\rho_V}}{\delta^{\alpha d+1}} = \frac{C_{\alpha,d,\rho_V}}{\rho_V^{\alpha d+1}} (2J+1)^{\alpha d+1}. \quad (3.10)$$

This piece of information will be used later in this proof.

On the other hand, denote for $j \in \mathbb{N}^*$,

$$\mathbf{G}_j^1 = \sum_{\{p+q+r=j|q \neq j\}} \mathbf{W} \frac{(ih\mathbf{V})^p}{p!} \mathbf{W}^* e^{-ih\Delta} S_q e^{ih\Delta} \mathbf{W} \frac{(-ih\mathbf{V})^r}{r!} \mathbf{W}^*,$$

$$\text{and} \quad \mathbf{G}_j^2 = - \sum_{\{p+q+r=j|q \neq j\}} \mathbf{Q}_p^* \mathbf{X}_q \mathbf{Q}_r,$$

the two members on the right hand side of equation (3.5). We have, as in [6] the estimates

$$\|\mathbf{G}_j^1\|_{(j)} \leq \tilde{C}^2 \sum_{\{p+q+r=j|q \neq j\}} \frac{(hM_V^{(3)})^{p+r}}{p!r!} \|\mathbf{S}_q\|_{(q+1)} \quad (3.11)$$

and

$$\|\mathbf{G}_j^2\|_{(j)} \leq \tilde{C}^2 \sum_{\{p+q+r=j|q \neq j\}} \|\mathbf{Q}_p\|_{(p)} \|\mathbf{X}_q\|_{(q)} \|\mathbf{Q}_r\|_{(r)}, \quad (3.12)$$

for the same constant \tilde{C} as above.

Besides, using Proposition 3.7 and setting $\kappa = \left(\frac{2\nu\alpha}{\delta}\right)^{2\nu\alpha} \frac{2^{2\nu} K^\nu}{\gamma h}$, we know that

$$\|\mathbf{S}_j\|_{(j+1)} \leq \kappa \left(\|\mathbf{G}_j^1\|_{(j)} + \|\mathbf{G}_j^2\|_{(j)} \right) \quad (3.13)$$

$$\text{and} \quad \|\mathbf{X}_j\|_j \leq \|\mathbf{G}_j^1\|_{(j)} + \|\mathbf{G}_j^2\|_{(j)}. \quad (3.14)$$

Therefore, setting

$$\mathbf{s}_0 = hM_V^{(3)} \kappa, \quad \mathbf{x}_0 = hM_V^{(3)} \quad \text{and} \quad \mathbf{q}_0 = 1,$$

and for all $j \in \mathbb{N}^*$,

$$\begin{aligned} \mathbf{s}_j &= \kappa \tilde{C}^2 \sum_{\{p+q+r=j|q \neq j\}} \left(\frac{(hM_V)^{p+r}}{p!r!} \mathbf{s}_q + \mathbf{q}_p \mathbf{q}_r \mathbf{x}_q \right), \\ \mathbf{q}_j &= \frac{\tilde{C}}{j} \sum_{k=0}^{j-1} \mathbf{q}_k \mathbf{s}_{j-k-1}, \\ \mathbf{x}_j &= \tilde{C}^2 \sum_{\{p+q+r=j|q \neq j\}} \left(\frac{(hM_V)^{p+r}}{p!r!} \mathbf{s}_q + \mathbf{q}_p \mathbf{q}_r \mathbf{x}_q \right), \end{aligned}$$

we recover the following estimates, valid for all $j \in \{0, \dots, J\}$,

$$\|\mathbf{S}_j\|_{(j+1)} \leq \mathbf{s}_j, \quad \|\mathbf{Q}_j\|_{(j)} \leq \mathbf{q}_j \quad \text{and} \quad \|\mathbf{X}_j\|_{(j)} \leq \mathbf{x}_j.$$

Second step.

There remains to estimate the terms \mathbf{s}_j , \mathbf{q}_j and \mathbf{x}_j , an independent task. To do so, we introduce as usual the associated power series expansions

$$\mathbf{s}(t) = \sum_{j \geq 0} \mathbf{s}_j t^j, \quad (3.15)$$

$$\mathbf{q}(t) = \sum_{j \geq 0} \mathbf{q}_j t^j, \quad (3.16)$$

$$\text{and } \mathbf{x}(t) = \sum_{j \geq 0} \mathbf{x}_j t^j. \quad (3.17)$$

The above relations between the \mathbf{s}_j 's, \mathbf{q}_j 's and \mathbf{x}_j 's transform into the following identities between $\mathbf{s}(t)$, $\mathbf{q}(t)$ and $\mathbf{x}(t)$, namely

$$\begin{aligned} \left(1 - \kappa \tilde{C}^2 (e^{2hM_V^{(3)}t} - 1)\right) \mathbf{s}(t) - \mathbf{s}_0 &= \kappa \tilde{C}^2 \mathbf{x}(t) (\mathbf{q}(t)^2 - 1), \\ \mathbf{q}'(t) &= \tilde{C} \mathbf{s}(t) \mathbf{q}(t), \\ \mathbf{x}(t) &= \kappa^{-1} \mathbf{s}(t). \end{aligned}$$

As a consequence, \mathbf{q} satisfies the following ordinary differential equation

$$\mathbf{q}'(t) = \frac{\mathbf{s}_0 \tilde{C} \mathbf{q}(t)}{1 - \tilde{C}^2 (\kappa (e^{2hM_V^{(3)}t} - 1) + (\mathbf{q}(t)^2 - 1))} \quad \text{and} \quad \mathbf{q}(0) = 1. \quad (3.18)$$

At this level of the analysis, we now invoke the independent and technical Lemma 5.1, whose proof is postponed to the last section. It provides that $0 \leq \mathbf{s}(t) \leq \frac{5\sqrt{5}}{4} \kappa h M_V^{(3)}$ whenever $0 \leq t < 1/16hM_V^{(3)} \kappa \tilde{C}^3$, which, using the standard Cauchy estimates for analytic functions, provides the following upper bound, valid for all $J \in \mathbb{N}^*$,

$$0 \leq \mathbf{s}_J \leq \frac{5\sqrt{5}}{4} \kappa h M_V^{(3)} (16hM_V^{(3)} \kappa \tilde{C}^3)^J = \frac{5\sqrt{5}}{4} 16^J \tilde{C}^{3J} (\kappa h M_V^{(3)})^{J+1}.$$

Now, taking into account the definition of κ , together with estimate (3.10) on \tilde{C} , yields

$$\mathbf{s}_J \leq C_1^J (2J+1)^{3(\alpha d+1)} \left[\left(\frac{2\nu\alpha}{\delta} \right)^{2\nu\alpha} \frac{2^{2\nu} K^\nu}{\gamma} \right]^{J+1},$$

where C_1 depends only on α, d, ρ_V and $M_V^{(3)}$. Hence,

$$\mathbf{s}_J \leq C_2^J (2J+1)^{3(\alpha d+1)} (2J+1)^{2\nu\alpha(J+1)} K^{\nu(J+1)},$$

where C_2 depends only on $\alpha, d, \rho_V, M_V^{(3)}, \nu$ and γ . Since $2J+1 \leq 3J$, and $J+1 \leq 2J$ we may write

$$\begin{aligned} \mathbf{s}_J &\leq C_3^J J^{3(\alpha d+1)+2\nu\alpha(J+1)} K^{2\nu J} \\ &\leq C_3^J J^{(3\alpha d+3+4\nu\alpha)J} K^{2\nu J}, \end{aligned}$$

where C_3 depends only on $\alpha, d, \rho_V, M_V^{(3)}, \nu$ and γ . The result follows since for all $J \in \mathbb{N}^*$,

$$\|\mathbf{S}_J\|_{\rho_V/2, \alpha} \leq \|\mathbf{S}_J\|_{(J+1)} \leq \mathbf{s}_J.$$

The proof is now complete. ■

3.4.2 Estimates on Σ and Q

Assume that $M \in \mathbb{N}$, $K > 0$ and $N > 0$ are given. Now that \mathbf{S}_n , \mathbf{X}_n and \mathbf{Q}_n have been cleanly constructed and estimated for all values of n , we define the following polynomials in $\lambda \in \mathbb{R}$:

$$\mathbf{S}^{[N]}(\lambda) = \sum_{0 \leq n \leq N} \lambda^n \mathbf{S}_n \quad \text{and} \quad \mathbf{X}^{[N]}(\lambda) = \sum_{0 \leq n \leq N} \lambda^n \mathbf{X}_n. \quad (3.19)$$

On the other hand, associated with $\mathbf{S}^{[N]}(\lambda)$ and $\mathbf{X}^{[N]}(\lambda)$, we reconstruct the two operators $\mathbf{Q}^{[N]}(\lambda)$ and $\Sigma^{[N]}(\lambda)$, defined as the solutions on \mathbb{R} to the following Cauchy problems

$$\begin{cases} i\partial_\lambda \mathbf{Q}^{[N]}(\lambda) = \mathbf{Q}^{[N]}(\lambda) \mathbf{S}^{[N]}(\lambda), \\ \mathbf{Q}^{[N]}(0) = \text{Id}_{(2M+1)^d}, \end{cases} \quad \text{and} \quad \begin{cases} i\partial_\lambda \Sigma^{[N]}(\lambda) = \Sigma^{[N]}(\lambda) \mathbf{X}^{[N]}(\lambda), \\ \Sigma^{[N]}(0) = e^{ih\Delta}. \end{cases} \quad (3.20)$$

It is an easy exercise to check that $\mathbf{Q}^{[N]}(\lambda)$ and $\Sigma^{[N]}(\lambda)$ are unitary. We introduce, for $\lambda \in \mathbb{R}$ sufficiently small, the following power series expansions

$$\mathbf{Q}^{[N]}(\lambda) = \sum_{n=0}^{+\infty} \mathbf{Q}_n^{[N]} \lambda^n \quad \text{and} \quad \Sigma^{[N]}(\lambda) = \sum_{n=0}^{+\infty} \Sigma_n^{[N]} \lambda^n.$$

It is fairly clear, comparing the respective power series expansions of the involved terms, that the following equalities hold between formal power series

$$\mathbf{S}^{[N]}(\lambda) = \mathbf{S}(\lambda) + \mathcal{O}(\lambda^{N+1}), \quad \mathbf{X}^{[N]}(\lambda) = \mathbf{X}(\lambda) + \mathcal{O}(\lambda^{N+1}),$$

and, more importantly,

$$\mathbf{Q}^{[N]}(\lambda) = \mathbf{Q}(\lambda) + \mathcal{O}(\lambda^{N+1}).$$

In particular, we immediately deduce that $\mathbf{S}^{[N]}(\lambda)$, $\mathbf{X}^{[N]}(\lambda)$, and $\mathbf{Q}^{[N]}(\lambda)$, solve the equation (3.4) to within $\mathcal{O}(\lambda^{N+1})$, in that the following relation holds true (between formal power series, and actually between normally convergent series)

$$\begin{aligned} \mathbf{S}^{[N]}(\lambda) - \mathbf{L}^*(\lambda) \mathbf{S}^{[N]}(\lambda) \mathbf{L}(\lambda) = \\ h \mathbf{W} \mathbf{V} \mathbf{W}^* - \left(\mathbf{Q}^{[N]}(\lambda) \right)^* \mathbf{X}^{[N]}(\lambda) \mathbf{Q}^{[N]}(\lambda) + \mathcal{O}(\lambda^{N+1}). \end{aligned} \quad (3.21)$$

There now remains to come back to the variables $\mathbf{Q}^{[N]}(\lambda)$ and $\Sigma^{[N]}(\lambda)$, and to prove that $\mathbf{Q}^{[N]}(\lambda) \mathbf{L}(\lambda) \mathbf{Q}^{[N]}(\lambda)^* = \Sigma^{[N]}(\lambda) + \mathcal{O}(\lambda^{N+1})$ as well. To do so, we introduce the remainder term

$$\mathbf{R}^{[N]}(\lambda) = \mathbf{Q}^{[N]}(\lambda) \mathbf{L}(\lambda) \mathbf{Q}^{[N]}(\lambda)^* - \Sigma^{[N]}(\lambda). \quad (3.22)$$

For later purposes, note that one can easily check we have the following expansion, valid in some neighborhood of $\lambda = 0$, and for all $M \in \mathbb{N}$,

$$\mathbf{R}^{[N]}(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \left[\sum_{p+q+r=n} \left(\mathbf{Q}_p^{[N]} e^{ih\Delta} \mathbf{W} \frac{(-ih)^q}{q!} \mathbf{V}^q \mathbf{W}^* (\mathbf{Q}_r^{[N]})^* \right) - \boldsymbol{\Sigma}_n^{[N]} \right], \quad (3.23)$$

an equality between converging series.

To prove that

$$\mathbf{R}^{[N]}(\lambda) = \mathcal{O}(\lambda^{N+1}),$$

we proceed in the same way we deduced relation (3.4) from (3.3). Differentiating relation $\mathbf{R}^{[N]}(\lambda) = \mathbf{Q}^{[N]}(\lambda) \mathbf{L}(\lambda) \mathbf{Q}^{[N]}(\lambda)^* - \boldsymbol{\Sigma}^{[N]}(\lambda)$ with respect to λ , using the relations $\mathbf{S}^{[N]}(\lambda) = i (\mathbf{Q}^{[N]})^* (\lambda) \partial_\lambda \mathbf{Q}^{[N]}(\lambda) = -i (\partial_\lambda \mathbf{Q}^{[N]}(\lambda))^* \mathbf{Q}^{[N]}(\lambda)$ (since $\mathbf{S}^{[N]}(\lambda)$ is hermitian) and similarly for $\mathbf{X}^{[N]}(\lambda)$ to remove all terms $\partial_\lambda \mathbf{Q}^{[N]}(\lambda)$ and $\partial_\lambda \boldsymbol{\Sigma}^{[N]}(\lambda)$, next using again the relation $\boldsymbol{\Sigma}^{[N]}(\lambda) = \mathbf{Q}^{[N]}(\lambda) \mathbf{L}(\lambda) (\mathbf{Q}^{[N]})^* (\lambda) - \mathbf{R}^{[N]}(\lambda)$, and lastly using the unitarity of $\mathbf{Q}^{[N]}(\lambda)$, $\mathbf{L}(\lambda)$ to factorize and eventually eliminate these terms whenever possible, we may establish that $\mathbf{X}^{[N]}(\lambda)$, $\mathbf{S}^{[N]}(\lambda)$ and $\mathbf{R}^{[N]}(\lambda)$ satisfy

$$\begin{aligned} i\partial_\lambda \mathbf{R}^{[N]}(\lambda) &= \mathbf{R}^{[N]}(\lambda) \mathbf{X}^{[N]}(\lambda) + \mathbf{Q}^{[N]}(\lambda) \mathbf{L}(\lambda) \left[(\mathbf{L}(\lambda))^* \mathbf{S}^{[N]}(\lambda) \mathbf{L}(\lambda) - \mathbf{S}^{[N]}(\lambda) \right. \\ &\quad \left. + (h\mathbf{W}\mathbf{V}\mathbf{W}^*) - (\mathbf{Q}^{[N]}(\lambda))^* \mathbf{X}^{[N]}(\lambda) \mathbf{Q}^{[N]}(\lambda) \right] (\mathbf{Q}^{[N]}(\lambda))^*. \end{aligned}$$

Hence, using relation (3.21) provides

$$i\partial_\lambda \mathbf{R}^{[N]}(\lambda) = \mathbf{R}^{[N]}(\lambda) \mathbf{X}^{[N]}(\lambda) + \mathcal{O}(\lambda^{N+1}),$$

which, using the initial value $\mathbf{R}^{[N]}(0) = 0$, eventually produces

$$\mathbf{R}^{[N]}(\lambda) = \mathcal{O}(\lambda^{N+1}).$$

As a conclusion, relation (3.23) reduces to

$$\mathbf{R}^{[N]}(\lambda) = \sum_{n \geq N+1}^{+\infty} \lambda^n \left[\sum_{p+q+r=n} \left(\mathbf{Q}_p^{[N]} e^{ih\Delta} \frac{(-ih)^q}{q!} \mathbf{W}\mathbf{V}^q \mathbf{W}^* (\mathbf{Q}_r^{[N]})^* \right) - \boldsymbol{\Sigma}_n^{[N]} \right]. \quad (3.24)$$

We are now in position to complete the estimates on $\mathbf{Q}^{[N]}(\lambda)$, $\boldsymbol{\Sigma}^{[N]}(\lambda)$, and $\mathbf{R}^{[N]}(\lambda)$.

3.4.3 Estimates for $\boldsymbol{\Sigma}^{[N]}$ and $\mathbf{Q}^{[N]}$

Lemma 3.10 *There exists a constant $C_1 \geq C_0$ depending only on V , $M_V^{(3)}$, ρ_V , α , γ , ν and d such that for all $N \geq 1$, all $n \in \mathbb{N}^*$, all $K \geq K_0$, all $h \in (0, 1)$ satisfying (3.6) and all $M \in \mathbb{N}$,*

$$\|\boldsymbol{\Sigma}_n^{[N]}\|_{\rho_V/4, \alpha} \leq h(C_1 K^{\mu_1} N^{\mu_2})^n \quad (3.25)$$

$$\text{and} \quad \|\mathbf{Q}_n^{[N]}\|_{\rho_V/4, \alpha} \leq (C_1 K^{\mu_2} N^{\mu_2})^n \quad (3.26)$$

where C_0 , K_0 , μ_1 and μ_2 are given in Proposition 3.9.

Proof. Since $\Sigma_0^{[N]} = e^{ih\Delta}$, we have $\|\Sigma_0^{[N]}\|_{\rho_V/4,\alpha} = 1$. Since $\Sigma_1^{[N]} = \Sigma_0^{[N]}\mathbf{X}_0$, we have by Corollary 2.6 and Lemma 2.7 that for all $M \in \mathbb{N}$, $\|\Sigma_1^{[N]}\|_{\rho_V/4,\alpha} \leq hM_V^{(3)}$. Assume now that (3.25) holds with some constant C_1 for all $k \in \{1, \dots, n\}$. By definition of $\Sigma^{[N]}$, Lemma 2.7, ensures that there exists a positive constant C depending on ρ_V and α such that

$$\|\Sigma_{n+1}^{[N]}\|_{\rho_V/4,\alpha} \leq \frac{C}{n+1} \sum_{k=0}^{\min(n,N)} \|\Sigma_{n-k}^{[N]}\|_{\rho_V/4,\alpha} \|\mathbf{X}_k\|_{\rho_V/3,\alpha}.$$

Using the induction hypothesis and the estimate (3.9), we get

$$\|\Sigma_{n+1}^{[N]}\|_{\rho_V/4,\alpha} \leq \frac{C}{n+1} \sum_{k=0}^{\min(n,N)} (C_1 K^{\mu_1} N^{\mu_2})^{n-k} h(C_0 K^{\mu_1} k^{\mu_2})^k.$$

If we assume that $C_1 \geq C_0$, we recover

$$\begin{aligned} \|\Sigma_{n+1}^{[N]}\|_{\rho_V/4,\alpha} &\leq h(C_1 K^{\mu_1} N^{\mu_2})^n \frac{C}{n+1} \sum_{k=0}^{\min(n,N)} \left(\frac{k}{N}\right)^{\mu_2 k} \\ &\leq h(C_1 K^{\alpha} N^{\beta})^n \frac{C}{n+1} \sum_{k=0}^{\min(n,N)} 1 \\ &\leq h(C_1 K^{\alpha} N^{\beta})^{n+1} \end{aligned}$$

provided $C_1 \geq C$ and since $K \geq 1$. This shows (3.25).

The proof of (3.26) is similar using the estimate (3.8) instead of (3.9). \blacksquare

The previous lemma yields the following proposition :

Proposition 3.11 *Using the previous notation, for all $K \geq K_0$, all $N \geq 1$, all $h \in (0, 1)$ satisfying (3.6), all $\lambda \in \mathbb{R}$ such that $|\lambda| \leq (2C_1 K^{\mu_1} N^{\mu_2})^{-1}$ and all $M \in \mathbb{N}$, we have*

$$\|\mathbf{Q}^{[N]}(\lambda) - \text{Id}_{(2M+1)^d}\|_{\rho_V/4,\alpha} \leq 2C_1 K^{\mu_1} N^{\mu_2} |\lambda| \quad (3.27)$$

and

$$\|\Sigma^{[N]}(\lambda) - e^{ih\Delta}\|_{\rho_V/4,\alpha} \leq 2hC_1 K^{\mu_1} N^{\mu_2} |\lambda|. \quad (3.28)$$

3.4.4 Estimate for the remainder term

Proposition 3.12 *Using the notations of Proposition 3.9, there exists a constant $C_2 > 0$ depending only on V , $M_V^{(3)}$, ρ_V , α , γ , ν and d such that for all $h \in (0, 1)$ satisfying (3.6), all $N \geq 1$, all $K \geq K_0$, all $\lambda \in \mathbb{R}$ such that $|\lambda| \leq (2C_1 K^{\mu_1} N^{\mu_2})^{-1}$ and all $M \in \mathbb{N}$, we have*

$$\|\mathbf{R}^{[N]}(\lambda)\|_{\rho_V/5,\alpha} \leq (C_2 |\lambda| K^{3\mu_1} N^{3(\mu_2+1)})^N. \quad (3.29)$$

Proof. Consider identity (3.24). Due to estimate (2.3) of Corollary 2.9 and estimates (3.25) and (3.26) of Lemma 3.10, and using Lemma 2.7, we observe that there exists a positive constant C depending only on ρ_V and α such that for all $h \in (0, 1)$ satisfying (3.6), all $N \geq 1$, all $K \geq K_0$, all $\lambda \in \mathbb{R}$ such that $|\lambda| \leq (2C_1 K^{\mu_1} N^{\mu_2})^{-1}$ and all $M \in \mathbb{N}$, we have

$$\begin{aligned} & \|\mathbf{R}^{[N]}(\lambda)\|_{\rho_V/5, \alpha} \\ & \leq C \sum_{n \geq N+1} |\lambda|^n \left[\sum_{p+q+r=n} \left((C_1 K^{\mu_1} N^{\mu_2})^p \frac{h^q}{q!} M_V^q (C_1 K^{\mu_1} N^{\mu_2})^r \right) \right] \\ & \quad + h \sum_{n \geq N+1} (|\lambda| C_1 K^{\mu_1} N^{\mu_2})^n. \end{aligned}$$

The result follows by standard calculus. See for example the proof of proposition 2.5.2 in [5]. \blacksquare

3.5 The normal form theorem

We are now able to state and prove the main result of our analysis.

Theorem 3.13 *Assume that V is a complex (ρ_V, α) -Gevrey fonction on \mathbb{T}^d . For all $M \in \mathbb{N}$, $\lambda \in \mathbb{R}$ and $h > 0$, consider the linear splitting operator*

$$\mathbf{L}(\lambda) = e^{ih\Delta} \mathbf{W} e^{-ih\mathbf{V}} \mathbf{W}^* = e^{ih\Delta} e^{-ih\mathbf{W}\mathbf{V}\mathbf{W}^*}.$$

Assume $\gamma > 0$ and $\nu > 1$ are given.

Then, there exist positive constants λ_0 , σ and c depending only on V , $M_V^{(3)}$, ρ_V , α , γ , ν and d such that for all timestep $h \in (0, 1)$ satisfying (3.6) and all $M \in \mathbb{N}$, there exist families of L^2 -unitary operators $\mathbf{Q}(\lambda)$ and $\mathbf{\Sigma}(\lambda)$ analytic in λ for $|\lambda| < \lambda_0$ such that for $\lambda \in (0, \lambda_0)$, the following equality holds

$$\mathbf{Q}(\lambda) \mathbf{L}(\lambda) \mathbf{Q}(\lambda)^* = \mathbf{\Sigma}(\lambda) + \mathbf{R}(\lambda), \quad (3.30)$$

where for all $M \in \mathbb{N}$, the remainder term $\mathbf{R}(\lambda)$ satisfies, for $\lambda \in (0, \lambda_0)$,

$$\|\mathbf{R}(\lambda)\|_{\rho_V/5, \alpha} \leq \exp(-c\lambda^{-\sigma}). \quad (3.31)$$

Besides, the following estimates hold true

$$\|\mathbf{Q}(\lambda) - \text{Id}_{(2M+1)^d}\|_{\rho_V/4, \alpha} \leq \lambda^{1/2} \quad \text{and} \quad \|\mathbf{\Sigma}(\lambda) - e^{ih\Delta}\|_{\rho_V/4, \alpha} \leq h\lambda^{1/2}. \quad (3.32)$$

Proof. As usual, the proof merely consists in gathering all previous estimates and choosing optimal values of the various truncation parameters.

Consider positive numbers σ_K and σ_N such that

$$\mu_1 \sigma_K + (\mu_2 + 1) \sigma_N \leq 1/4. \quad (3.33)$$

Since $\alpha \geq 1$, we have $\mu_2 \geq \mu_1$ and hence a possible choice for (σ_K, σ_N) is

$$\sigma_K = \sigma_N = \frac{1}{8 \max(\mu_1, \mu_2 + 1)} = \frac{1}{8(3\alpha d + 4(1 + \nu\alpha))}.$$

These parameters being now fixed, we set for all $\lambda \in (0, 1)$,

$$K = \lambda^{-\sigma_K} \quad \text{and} \quad N = \frac{1}{(2C_1)^{1/\mu_2}} \lambda^{-\sigma_N}, \quad (3.34)$$

and we define

$$\mathbf{Q}(\lambda) = \mathbf{Q}^{[N]}(\lambda), \quad \mathbf{\Sigma}(\lambda) = \mathbf{\Sigma}^{[N]}(\lambda) \quad \text{and} \quad \mathbf{R}(\lambda) = \mathbf{R}^{[N]}(\lambda).$$

By Proposition 3.10, C_1 only depends on V , $M^{(3)}$, ρ_V , α , ν , γ and d . Hence, there exists a positive constant $\lambda_0 \in (0, 1)$ depending only on these parameters such that for all $\lambda \in (0, \lambda_0)$, we have $K = \lambda^{-\sigma_K} \geq K_0$ and $N = 1/(2C_1)^{1/\mu_2} \lambda^{-\sigma_N} \geq 1$. For such a λ , we have

$$(2C_1 K^{\mu_1} N^{\mu_2})^{-1} = \lambda^{\mu_1 \sigma_K + \mu_2 \sigma_N} \geq \lambda$$

since $\mu_1 \sigma_K + \mu_2 \sigma_N \leq 1$ with (3.33) and $\lambda \in (0, 1)$.

Therefore, Proposition 3.11 ensures that for all $\lambda \in (0, \lambda_0)$ and all $M \in \mathbb{N}$,

$$\|\mathbf{Q}(\lambda) - \text{Id}\|_{\rho_V/4, \alpha} \leq \lambda^{1-(\alpha\sigma_K + \mu_2\sigma_N)} \leq \lambda^{1/2}$$

and

$$\|\mathbf{\Sigma}(\lambda) - e^{ih\Delta}\|_{\rho_V/4, \alpha} \leq h\lambda^{1-(\alpha\sigma_K + \mu_2\sigma_N)} \leq h\lambda^{1/2}.$$

Moreover, Proposition 3.12 ensures that

$$\|\mathbf{R}(\lambda)\|_{\rho_V/5, \alpha} \leq (C_2 C_1^{-3(\mu_2+1)/\mu_2} \lambda^{1-(3\alpha\sigma_K + 3(\mu_2+1)\sigma_N)})^N.$$

As the exponent of λ in the right hand side of this inequality satisfies

$$1 - (3\mu_1\sigma_K + 3(\mu_2 + 1)\sigma_N) \geq 1/4 > 0$$

by (3.33), after a possible decrease of λ_0 (depending only on V , $M_V^{(3)}$, ρ_V , α , γ , ν and d again¹), we can assume that

$$\forall \lambda \in (0, \lambda_0) \quad C_2 C_1^{-3(\mu_2+1)/\mu_2} \lambda^{1-(3\mu_1\sigma_K + 3(\mu_2+1)\sigma_N)} \leq e^{-1}.$$

Therefore, we get eventually that for all $\lambda \in (0, \lambda_0)$ and all $M \in \mathbb{N}$,

$$\|\mathbf{R}(\lambda)\|_{\rho_V/5, \alpha} \leq e^{-N} = e^{\frac{-1}{(2C_1)^{1/\mu_2}} \lambda^{-\sigma_N}}.$$

This concludes the proof with $\sigma = \sigma_N = \sigma_K$. ■

4 Consequences of the normal form theorem

This section is devoted to drawing various consequences of our normal form theorem. Our main result is Theorem 4.10 below. We prove here that the numerical

¹We recall that C_2 only depends on V , $M_V^{(3)}$, ρ_V , α , γ , ν and d by Proposition 3.12

solution of the linear Schrödinger equation (3.2) computed using the symplectic splitting propagator (3.1) keeps Gevrey smoothness over exponentially long times. This may be seen as the central result of the present paper.

4.1 Spatial discretization

This short paragraph is devoted to some preliminary results relating Gevrey regularity of functions with the smoothness of their spatial discretization obtained *via* the Fast Fourier Transform algorithm.

As we did for V in Section 2.2, for all complex function $u \in L^1(\mathbb{T}^d)$ and all $M \in \mathbb{N}$, we consider the following vector $\mathbf{u} \in \mathbb{C}^{(2M+1)^d}$ approximating the Fourier coefficients of u :

$$\forall n \in \mathcal{B}_M, \quad \mathbf{u}_n = \frac{1}{(2M+1)^d} \sum_{p \in \mathcal{B}_M} u(x_p) e^{-inx_p}. \quad (4.1)$$

Definition 4.1 *For all $M \in \mathbb{N}$, all $\rho > 0$ and all $\alpha \geq 1$, the complex vector space $\mathbb{C}^{(2M+1)^d}$ is endowed with the norm defined for all $\mathbf{u} \in \mathbb{C}^{(2M+1)^d}$ by*

$$\|\mathbf{u}\|_{\rho, \alpha} = \sup \{ |\mathbf{u}_n| e^{\rho|n|^{1/\alpha}} \mid n \in \mathcal{B}_M \}.$$

Definition 4.2 *For all $\rho > 0$ and all $\alpha \geq 1$, the complex vector space of (ρ, α) -Gevrey functions is endowed with the norm defined by*

$$\|u\|_{\rho, \alpha} = \sup \{ |\hat{u}_n| e^{\rho|n|^{1/\alpha}} \mid n \in \mathbb{Z}^d \}.$$

We will use the following approximation result:

Lemma 4.3 *Set $\rho > 0$ and $\alpha \geq 1$. For all $\mu \in (0, \rho)$, there exists a positive constant C depending only on ρ, μ, α and d such that for all complex function u in the class of (ρ, α) -Gevrey functions, we have*

$$\forall M \in \mathbb{N}, \forall n \in \mathcal{B}_M, \quad \|\mathbf{u}\|_{\mu, \alpha} \leq C \|u\|_{\rho, \alpha}.$$

Proof. Adapting the proof of Lemma 2.4 and replacing V by u in this proof, which is allowed since the function $u = V$ is (ρ_V, α) -Gevrey provided $\rho = \rho_V$, we get that for all $M \in \mathbb{N}$, all $n \in \mathcal{B}_M$,

$$\begin{aligned} |(\hat{g}_n)_n| &\leq 2|n| |\hat{u}_n| \leq 2\|u\|_{\rho, \alpha} |n| e^{-\rho|n|^{1/\alpha}} \\ &\leq 2\|u\|_{\rho, \alpha} |n| e^{-(\rho-\mu)|n|^{1/\alpha}} e^{-\mu|n|^{1/\alpha}} \leq C_1 \|u\|_{\rho, \alpha} e^{-\mu|n|^{1/\alpha}}, \end{aligned}$$

with $C_1 = 2 \sup_{p \in \mathbb{Z}^d} |p| e^{-(\rho-\mu)|p|^{1/\alpha}}$. Hence,

$$\forall M \in \mathbb{N}, \forall n \in \mathcal{B}_M, \quad |\mathbf{u}_n - \hat{u}_n| \leq C_1 \frac{2\pi}{2M+1} \|u\|_{\rho, \alpha} e^{-\mu|n|^{1/\alpha}}.$$

This yields for all $M \in \mathbb{N}$ and $n \in \mathcal{B}_M$,

$$|\mathbf{u}_n| e^{\mu|n|^{1/\alpha}} \leq |\hat{u}_n| e^{\mu|n|^{1/\alpha}} + C_1 \frac{2\pi}{2M+1} \|u\|_{\rho, \alpha}.$$

The result follows. ■

For later purposes, we now define two additional ℓ^2 -norms on vectors \mathbf{u} . In what follows, the norm $\|\mathbf{u}\|$ may be seen as the total energy (or mass) of \mathbf{u} , while $|\mathbf{u}|_{|k|}$ is the energy of \mathbf{u} carried by Fourier modes p such that $|p| = |k|$. In other words, it is the energy carried by spatial frequencies of size $|k|$.

Definition 4.4 *For all $M \in \mathbb{N}$, $k = (k_1, \dots, k_d) \in \mathbb{Z}^d$ and $\mathbf{u} \in \mathbb{C}^{(2M+1)^d}$, we define*

$$|\mathbf{u}|_{|k|} = \sqrt{\sum_{p \in \mathbb{Z}^d \text{ s.t. } |p|=|k|} |\mathbf{u}_p|^2},$$

and

$$\|\mathbf{u}\| = \sqrt{\sum_{p \in \mathcal{B}_M} |\mathbf{u}_p|^2}.$$

Lemma 4.5 *For all $\rho > 0$ and all $\alpha \geq 1$, there exists a positive constant $C_{\rho, \alpha}$ depending only on ρ and α such that for all $M \in \mathbb{N}$, for all linear operator \mathbf{R} on $\mathbb{C}^{(2M+1)^d}$ and all vector $\mathbf{u} \in \mathbb{C}^{(2M+1)^d}$, we have*

$$\forall k \in \mathcal{B}_M, \quad |(\mathbf{R}\mathbf{u})_k| \leq |\mathbf{R}\mathbf{u}|_{|k|} \leq \|\mathbf{R}\mathbf{u}\| \leq C_{\rho, \alpha} \|\mathbf{R}\|_{\rho, \alpha} \|\mathbf{u}\|.$$

4.2 Conservation of the regularity over long times

4.2.1 The time iteration

For a complex function $u_0 \in L^1(\mathbb{T}^d)$ and for all $M \in \mathbb{N}$, we consider the following method, defined for the timestep $h > 0$ for all $\lambda \in \mathbb{R}$ by

$$\forall n \in \mathbb{N}, \quad \mathbf{u}^n = \mathbf{L}(\lambda)^n \mathbf{u}_0,$$

where \mathbf{u}_0 is the discretization of order M of u_0 defined by Formula (4.1).

For all fixed $M \in \mathbb{N}$, we prove conservation of the Gevrey regularity of the so-obtained numerical solution over exponentially long times. Our approach relies on the normal form Theorem we proved above, and the regularity is actually measured by exploiting a change of variables based on the matrix $\mathbf{Q}(\lambda)$. Note that high modes (see Lemma 4.7) and low modes (see Lemma 4.6) in the new variables are treated differently.

Let us come to quantitative statements. For $|\lambda| < \lambda_0$, we use the change of variables (3.30) by setting for all $M \in \mathbb{N}$,

$$\forall n \in \mathbb{N}, \quad \mathbf{v}^n = \mathbf{Q}(\lambda) \mathbf{u}^n.$$

To distinguish high modes from low modes, we set for all $M \in \mathbb{N}$, $K > 0$ and $\mathbf{u} \in \mathbb{C}^{(2M+1)^d}$,

$$(\pi_K(\mathbf{u}))_k = \begin{cases} 0 & \text{if } |k| \leq K \\ \mathbf{u}_k & \text{otherwise.} \end{cases} \quad (4.2)$$

Hence, for all $K > 0$, π_K is a linear projection operator on $\mathbb{C}^{(2M+1)^d}$.

4.2.2 Conservation for low modes

We have the following conservation result for the low modes in the new variables:

Lemma 4.6 *There exists a positive constant C_{low} depending only on V , $M_V^{(3)}$, ρ_V , α , γ , ν and d such that for all $\lambda \in (0, \lambda_0)$, all $M \in \mathbb{N}$, all $h \in (0, 1)$ satisfying (3.6), and all $n \leq e^{c\lambda^{-\sigma}/2}$, we have*

$$\forall k \in \mathbb{Z}^d \text{ s.t. } |k| \leq \lambda^{-\sigma}, \quad \left| |\mathbf{v}^n|_{|k|} - |\mathbf{v}^0|_{|k|} \right| \leq C_{low} e^{-c\lambda^{-\sigma}/2} \|\mathbf{u}_0\|. \quad (4.3)$$

Proof. The unitarity of $\mathbf{L}(\lambda)$ and $\mathbf{Q}(\lambda)$ ensures that

$$\forall n \in \mathbb{N}, \quad \|\mathbf{u}^n\| = \|\mathbf{v}^n\|.$$

Since $\Sigma(\lambda)$ is unitary and almost-X-shaped, we have for all $k \in \mathbb{Z}^d$ such that $|k| \leq K = \lambda^{-\sigma}$,

$$|\mathbf{u}^n|_{|k|} = |\Sigma(\lambda)\mathbf{u}^n|_{|k|}. \quad (4.4)$$

Hence,

$$\begin{aligned} \left| |\mathbf{u}^{n+1}|_{|k|} - |\mathbf{u}^n|_{|k|} \right| &\leq \left| |\mathbf{u}^{n+1}|_{|k|} - |\Sigma(\lambda)\mathbf{u}^n|_{|k|} \right| \\ &\leq \left| \mathbf{u}^{n+1} - \Sigma(\lambda)\mathbf{u}^n \right|_{|k|} \\ &\leq |\mathbf{R}(\lambda)\mathbf{u}^n| \\ &\leq C_{\rho_V/5, \alpha} \|\mathbf{R}(\lambda)\|_{\rho_V/5, \alpha} \|\mathbf{u}^n\| \\ &\leq C_{\rho_V/5, \alpha} e^{-c\lambda^{-\sigma}} \|\mathbf{u}_0\|, \end{aligned}$$

where we have used Lemma 4.5, Theorem 3.13 and Relation (4.4).

The result follows. ■

4.2.3 Conservation for high modes

The same kind of ideas yields conservation of smoothness for the high modes in the new variables:

Lemma 4.7 *There exists a positive constant C_{high} depending only on V , $M_V^{(3)}$, ρ_V , α , γ , ν and d such that for all $\lambda \in (0, \lambda_0)$, all $M \in \mathbb{N}$, all $h \in (0, 1)$ satisfying (3.6), and all $n \leq e^{c\lambda^{-\sigma}/2}$, we have*

$$\left| \|\pi_{\lambda^{-\sigma}} \mathbf{v}^n\| - \|\pi_{\lambda^{-\sigma}} \mathbf{v}^0\| \right| \leq C_{high} e^{-c\lambda^{-\sigma}/2} \|\mathbf{u}_0\|. \quad (4.5)$$

Proof. For all $\lambda \in (0, \lambda_0)$, we set $K = \lambda^{-\sigma} > 0$. Since $\Sigma(\lambda)$ is unitary and almost-X-shaped, we have

$$\forall \mathbf{u} \in \mathbb{C}^{(2M+1)^d}, \quad \|\pi_K(\mathbf{u})\| = \|\pi_K(\Sigma(\lambda)\mathbf{u})\|. \quad (4.6)$$

Hence,

$$\begin{aligned}
\left| \|\pi_K(\mathbf{v}^{n+1})\| - \|\pi_K(\mathbf{v}^n)\| \right| &\leq \left| \|\pi_K(\mathbf{v}^{n+1})\| - \|\pi_K(\Sigma(\lambda)\mathbf{v}^n)\| \right| \\
&\leq \|\pi_K(\mathbf{v}^{n+1} - \Sigma(\lambda)\mathbf{v}^n)\| \\
&\leq \|\pi_K(\mathbf{R}(\lambda)\mathbf{v}^n)\| \\
&\leq C_{\rho_V/5, \alpha} \|\mathbf{R}(\lambda)\|_{\rho_V/5, \alpha} \|\mathbf{v}^n\| \\
&\leq C_{\rho_V/5, \alpha} e^{-c\lambda^{-\sigma}} \|\mathbf{v}_0\|,
\end{aligned}$$

where we used Lemma 4.5, Theorem 3.13 and Relation (4.4).

The result follows. \blacksquare

4.2.4 Back to the original variables

We now gather the information obtained on low and high modes, to produce our final result, namely Theorem 4.10 below.

To do so, we need some technical tools. Firstly, for all $\lambda \in (0, \lambda_0)$ and all $k \in \mathbb{Z}^d$ such that $|k| \leq \lambda^{-\sigma}$, we shall make repeated use of the following inequality

$$| |\mathbf{u}^n|_{|k|} - |\mathbf{u}^0|_{|k|} | \leq | |\mathbf{u}^n|_{|k|} - |\mathbf{v}^n|_{|k|} | + | |\mathbf{v}^n|_{|k|} - |\mathbf{v}^0|_{|k|} | + | |\mathbf{v}^0|_{|k|} - |\mathbf{u}^0|_{|k|} |. \quad (4.7)$$

Secondly, we shall also use the two following lemmas:

Lemma 4.8 *For all $\rho, \delta > 0$ and $\alpha \geq 1$, there exists a positive constant C such that for all $M \in \mathbb{N}$, for all linear operator \mathbf{A} on $\mathbb{C}^{(2M+1)^d}$, for all $\mathbf{u} \in \mathbb{C}^{(2M+1)^d}$, we have*

$$\|\mathbf{A}\mathbf{u}\|_{\rho, \alpha} \leq C \|\mathbf{A}\|_{\rho+\delta, \alpha} \|\mathbf{u}\|_{\rho, \alpha}.$$

Proof. For all $k \in \mathcal{B}_M$,

$$\begin{aligned}
|(\mathbf{A}\mathbf{u})_k| e^{+\rho|k|^{1/\alpha}} &\leq \|\mathbf{A}\|_{\rho, \alpha} \|\mathbf{u}\|_{\rho, \alpha} \sum_{\ell \in \mathcal{B}_M} e^{-\delta|k-\ell|^{1/\alpha}} \underbrace{e^{-\rho|k-\ell|^{1/\alpha}} e^{-\rho|\ell|^{1/\alpha}} e^{+\rho|k|^{1/\alpha}}}_{\leq 1} \\
&\leq \left(\sum_{\ell \in \mathbb{Z}^d} e^{-\delta|\ell|^{1/\alpha}} \right) \|\mathbf{A}\|_{\rho, \alpha} \|\mathbf{u}\|_{\rho, \alpha}.
\end{aligned}$$

\blacksquare

Lemma 4.9 *For all $\rho, \delta > 0$ and $\alpha \geq 1$, there exists a positive constant C such that*

$$\forall M \in \mathbb{N}, \forall \mathbf{u} \in \mathbb{C}^{(2M+1)^d}, \quad \sup_{k \in \mathcal{B}_M} |\mathbf{u}|_{|k|} e^{\rho|k|^{1/\alpha}} \leq C \|\mathbf{u}\|_{\rho+\delta, \alpha}.$$

Proof. For all such M and \mathbf{u} , we have for all $k \in \mathcal{B}_M$,

$$\begin{aligned}
|\mathbf{u}|_{|k|}^2 e^{2\rho|k|^{1/\alpha}} &\leq e^{2\rho|k|^{1/\alpha}} \sum_{p \in \mathcal{B}_M \text{ s.t. } |p|=|k|} |\mathbf{u}_k|^2 \\
&\leq e^{2\rho|k|^{1/\alpha}} \sum_{p \in \mathcal{B}_M \text{ s.t. } |p| \leq |k|} |\mathbf{u}_k|^2 \\
&\leq e^{-2\delta|k|^{1/\alpha}} \sum_{p \in \mathcal{B}_M \text{ s.t. } |p|_\infty \leq |k|} |\mathbf{u}_k|^2 e^{2(\rho+\delta)|k|^{1/\alpha}} \\
&\leq e^{-2\delta|k|^{1/\alpha}} (2|k| + 1)^d \|\mathbf{u}\|_{\rho+\delta, \alpha}^2.
\end{aligned}$$

This concludes the proof with $C = \sup_{x \geq 0} e^{-\delta x^{1/\alpha}} (2x + 1)^{d/2}$. \blacksquare

We are now able to prove the

Theorem 4.10 *There exists a positive constant μ_0 depending only on V , $M_V^{(3)}$, ρ_V , α , γ , ν , d and λ_0 such that for all $\rho \in (0, \rho_V/5)$, and all $\mu \in (0, \mu_0)$, there exists a positive constant C such that for all $\lambda \in (0, \lambda_0)$, all $h \in (0, 1)$ satisfying (3.6), all $n \leq e^{c\lambda^{-\sigma}/2}$, we have*

$$\forall M \in \mathbb{N}, \quad \sup_{k \in \mathcal{B}_M \text{ s.t. } k \leq \lambda^{-\sigma}} \left| |\mathbf{u}^n|_{|k|} - |\mathbf{u}^0|_{|k|} \right| e^{\mu|k|^{1/\alpha}} \leq C \lambda^{1/2} \|\mathbf{u}_0\|_{\rho, \alpha}. \quad (4.8)$$

Proof. By Lemma 4.6, we have for all $\lambda \in (0, \lambda_0)$, all $h \in (0, 1)$ satisfying (3.6), all $k \in \mathcal{B}_M$ such that $|k| \leq \lambda^{-\sigma}$, all $n \leq e^{-c\lambda^{-\sigma}/2}$, and all $\mu > 0$,

$$\left| |\mathbf{v}^n|_{|k|} - |\mathbf{v}^0|_{|k|} \right| e^{+\mu|k|^{1/\alpha}} \leq C_{low} \exp\left((\mu - c/2)\lambda^{-\frac{\sigma}{\alpha}}\right) \|\mathbf{u}_0\|.$$

To take into account the two other terms in the right hand side of Relation (4.7), we note that

$$\begin{aligned}
\left| |\mathbf{u}^n|_{|k|} - |\mathbf{v}^n|_{|k|} \right| &\leq |\mathbf{u}^n - \mathbf{v}^n|_{|k|} \\
&\leq |(\text{Id} - \mathbf{Q}^*(\lambda))\mathbf{v}^n|_{|k|}.
\end{aligned}$$

We derive that this quantity is bounded by

$$\left| (\text{Id} - \mathbf{Q}^*(\lambda))\pi_{\lambda^{-\sigma}}\mathbf{v}^n \right|_{|k|} + \left| (\text{Id} - \mathbf{Q}^*(\lambda))(\text{Id} - \pi_{\lambda^{-\sigma}})\mathbf{v}^n \right|_{|k|}. \quad (4.9)$$

Lemma 4.7 ensures that

$$\|\pi_{\lambda^{-\sigma}}\mathbf{v}^n\| \leq \|\pi_{\lambda^{-\sigma}}\mathbf{Q}(\lambda)\mathbf{u}^0\| + C_{high}e^{-c\lambda^{-\sigma}}\|\mathbf{u}_0\|. \quad (4.10)$$

Lemma 4.8 and Theorem 3.13 ensure that $\|\mathbf{Q}(\lambda)\mathbf{u}_0\|_{\rho, \alpha} \leq C(1 + \lambda_0^{1/2})\|\mathbf{u}_0\|_{\rho, \alpha}$,

where C only depends on ρ , δ and α . Hence,

$$\begin{aligned}
\|\pi_{\lambda^{-\sigma}} \mathbf{Q}(\lambda) \mathbf{u}^0\|^2 &= \sum_{k \in \mathcal{B}_M \text{ s.t. } |k| > \lambda^{-\sigma}} |(\mathbf{Q}(\lambda) \mathbf{u}^0)_k|^2 \\
&\leq \|\mathbf{Q}(\lambda) \mathbf{u}^0\|_{\rho, \alpha}^2 \sum_{|k| > \lambda^{-\sigma}} e^{-2\rho|k|^{1/\alpha}} \\
&\leq \|\mathbf{Q}(\lambda) \mathbf{u}^0\|_{\rho, \alpha}^2 \sum_{k \in \mathbb{Z}^d \text{ s.t. } |k|_\infty > \lambda^{-\sigma}/d} e^{-2\rho|k|_\infty^{1/\alpha}} \\
&\leq \|\mathbf{Q}(\lambda) \mathbf{u}^0\|_{\rho, \alpha}^2 \sum_{p \in \mathbb{N} \text{ s.t. } p > \lambda^{-\sigma}/d} (2p+1)^d e^{-2\rho p^{1/\alpha}} \\
&\leq C^2 \|\mathbf{Q}(\lambda) \mathbf{u}^0\|_{\rho, \alpha}^2 \sum_{p \in \mathbb{N} \text{ s.t. } p > \lambda^{-\sigma}/d} \frac{2(\rho-\delta)}{\alpha} p^{1/\alpha-1} e^{2(\delta-\rho)p^{1/\alpha}} \\
&\leq C^2 \|\mathbf{Q}(\lambda) \mathbf{u}^0\|_{\rho, \alpha}^2 \int_{\lfloor \frac{\lambda^{-\sigma}}{d} \rfloor}^{\infty} \frac{2(\rho-\delta)}{\alpha} x^{1/\alpha-1} e^{2(\delta-\rho)x^{1/\alpha}} dx \\
&\leq C^2 (1 + \lambda_0^{1/2})^2 \|\mathbf{u}_0\|_{\rho, \alpha}^2 e^{2(\delta-\rho)[\lambda^{-\sigma}/d]^{1/\alpha}},
\end{aligned}$$

provided $\lambda_0^{-\sigma/\alpha} \geq \frac{d\alpha}{2\rho} + 1$, and with $C > 0$ such that

$$\forall x > \lambda_0^{-\sigma}/d, \quad (2x+1)^d \leq C^2 \frac{2(\rho-\delta)}{\alpha} x^{1/\alpha-1} e^{2\delta x^{1/\alpha}},$$

depending only on α , ρ , δ , d and λ_0 .

Using (4.10), we derive that there exists $\mu_0 \in (0, \rho)$ and $C_0, c_0 > 0$ depending only on V , ρ_V , α , γ , ν and d such that for all $n \leq e^{c\lambda^{-\sigma}/2}$ and all $h \in (0, 1)$ satisfying (3.6), we have for all $M \in \mathbb{N}$ and all $\mu \in (0, \mu_0)$

$$\forall k \in \mathcal{B}_M \text{ s.t. } |k| \leq \lambda^{-\sigma}, \quad \|\pi_{\lambda^{-\sigma}} \mathbf{v}^n\| e^{+\mu|k|^{1/\alpha}} \leq C_0 e^{-c_0(\mu_0-\mu)\lambda^{-\frac{\sigma}{\alpha}}} \|\mathbf{u}_0\|_{\rho, \alpha}.$$

By Lemma 4.5, we derive that

$$\|(\text{Id} - \mathbf{Q}^*(\lambda)) \pi_{\lambda^{-\sigma}} \mathbf{v}^n\|_{|k|} e^{\mu|k|^{1/\alpha}} \leq C_1 \lambda^{1/2} \|\mathbf{u}_0\|_{\rho, \alpha} \quad (4.11)$$

Choose $\mu \in (0, \mu_0)$ and $\delta > 0$ such that $\mu + 2\delta < \mu_0$. For all $k \in \mathcal{B}_M$ such that $|k| \leq \lambda^{-\sigma}$ and all $n \geq e^{-c\lambda^{-\sigma}/2}$, we have by Lemma 4.9, Lemma 4.8 and Theorem 3.13

$$\begin{aligned}
\|(\text{Id} - \mathbf{Q}^*(\lambda))(\text{Id} - \pi_{\lambda^{-\sigma}}) \mathbf{v}^n\|_{|k|} e^{\mu|k|^{1/\alpha}} &\leq C \|(\text{Id} - \mathbf{Q}^*(\lambda))(\text{Id} - \pi_{\lambda^{-\sigma}}) \mathbf{v}^n\|_{\mu+\delta, \alpha} \\
&\leq C \lambda^{1/2} \|(\text{Id} - \pi_{\lambda^{-\sigma}}) \mathbf{v}^n\|_{\mu+\delta, \alpha}.
\end{aligned}$$

Moreover, by Definition 4.1, Lemma 4.6 and Lemma 4.9, we get

$$\begin{aligned}
\|(\text{Id} - \pi_{\lambda^{-\sigma}})\mathbf{v}^n\|_{\mu+\delta,\alpha} &\leq \sup_{k \in \mathcal{B}_M \text{ s.t. } |k| \leq \lambda^{-\sigma}} |\mathbf{v}^n|_{|k|} e^{(\mu+\delta)|k|^{1/\alpha}} \\
&\leq \sup_{k \in \mathcal{B}_M \text{ s.t. } |k| \leq \lambda^{-\sigma}} |\mathbf{v}^0|_{|k|} e^{(\mu+\delta)|k|^{1/\alpha}} + C_{low} e^{(\mu+\delta-c/2)\lambda^{-\sigma}} \|\mathbf{u}_0\| \\
&\leq C \|\mathbf{v}_0\|_{\mu+2\delta,\alpha} + C_{low} e^{(\mu+\delta-c/2)\lambda^{-\sigma}} \|\mathbf{u}_0\| \\
&\leq C(1 + \lambda_0^{1/2}) \|\mathbf{u}_0\|_{\mu+2\delta,\alpha} + C_{low} e^{(\mu+\delta-c/2)\lambda^{-\sigma}} \|\mathbf{u}_0\|.
\end{aligned}$$

We deduce that, for some positive constant C_2 , we have

$$|(\text{Id} - \mathbf{Q}^*(\lambda))(\text{Id} - \pi_{\lambda^{-\sigma}})\mathbf{v}^n|_{|k|} e^{\mu|k|^{1/\alpha}} \leq C_2 \lambda^{1/2} \|\mathbf{u}_0\|_{\rho,\alpha}, \quad (4.12)$$

since $\mu + 2\delta < \mu_0 < \rho$. Using relation (4.9), we deduce that for all $n \leq e^{c\lambda^{-\sigma}/2}$, we have

$$\forall k \in \mathcal{B}_M \text{ s.t. } |k| \leq \lambda^{-\sigma}, \quad \left| |\mathbf{u}^n|_{|k|} - |\mathbf{v}^n|_{|k|} \right| e^{\mu|k|^{1/\alpha}} \leq C \lambda^{1/2} \|\mathbf{u}_0\|_{\rho,\alpha}.$$

We conclude the proof by using relation (4.7). ■

Remark 4.11 *Using Lemma 4.3, one can change $\|\mathbf{u}_0\|_{\rho,\alpha}$ to $\|u_0\|_{\rho,\alpha}$ without modifying the statement of Theorem 4.10.*

5 Technical Lemmas

This section is a mere collection of technical lemmas used in the course of the proof of our normal form Theorem. We simply state and prove these lemmas, without further comment.

Lemma 5.1 *Using the notation of Proposition 3.9 and its proof, let us define*

$$K_0 = \max \left(1, \left(\frac{\rho_V}{2\alpha\nu} \right)^{2\alpha} \gamma^{1/\nu} \right) \quad \text{and} \quad r^{-1} = 16hM_V^{(3)} \kappa \tilde{C}^3.$$

For all $K \geq K_0$ and $h \in (0, 1)$ satisfying (3.6), the functions \mathbf{x} , \mathbf{q} and \mathbf{s} defined by (3.15), (3.16) and (3.17) are analytic in $(-r, r)$, and satisfy for all $t \in (-r, r)$ the estimates:

$$0 < \mathbf{s}(t) \leq \frac{5\sqrt{5}}{4} \kappa h M_V^{(3)}, \quad 0, 8 < \mathbf{q}(t) \leq \frac{\sqrt{5}}{2} \quad \text{and} \quad 0 < \mathbf{x}(t) \leq \frac{5\sqrt{5}}{4} h M_V^{(3)}.$$

Proof. We consider the differential equation

$$\begin{cases} \mathbf{q}'(t) &= f(t, \mathbf{q}(t)) \\ \mathbf{q}(0) &= 1 \end{cases}$$

with

$$f(t, Y) = \frac{\mathbf{s}_0 \tilde{C} Y}{1 - \tilde{C}^2 (\kappa (e^{2hM_V^{(3)}t} - 1) + (Y^2 - 1))}$$

(recall that $\mathbf{s}_0 = M_V^{(3)} \kappa h$).

This equation has a unique analytical solution: there exists a number $R > 0$ such that for $t \in (-R, R)$, $\mathbf{q}(t)$ expands in power series of t . We can assume that R is maximal in this sense.

Due to the singularity in the denominator of $f(t, Y)$, define the two truncation parameters

$$T = \frac{1}{2hM_V^{(3)}} \ln \left(1 + \frac{1}{4\kappa\tilde{C}^2} \right) \quad \text{and} \quad D = \left(1 + \frac{1}{4\tilde{C}^2} \right)^{1/2} - 1.$$

Whenever $0 \leq t \leq T$ we have $\tilde{C}^2 \kappa (e^{2hM_V^{(3)}t} - 1) \leq \frac{1}{4}$. Besides, whenever $1 \leq Y \leq 1 + D$, we also have $\tilde{C}^2(Y^2 - 1) \leq \frac{1}{4}$. Therefore,

$$\begin{cases} 0 \leq t \leq T \\ 1 \leq Y \leq 1 + D \end{cases} \implies 0 < f(t, Y) \leq 2\mathbf{s}_0 \tilde{C}(D + 1). \quad (5.1)$$

This implies that \mathbf{q} is an increasing function of t as long as $t \in (0, T)$ and $1 \leq \mathbf{q}(t) \leq D + 1$. Note that, for $t \leq 0$, we have $0 < \mathbf{q}(t) \leq 1$. Note also, using the bound $\ln(1 + x) \geq \frac{1}{2}x$ whenever $0 \leq x \leq 1$, that we have

$$T = \frac{1}{2hM_V^{(3)}} \ln \left(1 + \frac{1}{4\kappa\tilde{C}^2} \right) \geq \frac{1}{16hM_V^{(3)}\kappa\tilde{C}^2}. \quad (5.2)$$

(Here we used the fact that the constraint $K \geq K_0$ together with the chosen value of K_0 , and that of κ , ensure the lower bound $\kappa \geq 1/4$).

Let us now examine the domain of validity of the bound $\mathbf{q}(t) \leq 1 + D$. To begin with, assume that for all $t \in (0, R)$, $1 < \mathbf{q}(t) < 1 + D$. In that case we necessarily have the relation $T < R$. Alternatively, assume that there exists $0 < t_D^* < R$ such that $\mathbf{q}(t_D^*) = 1 + D$. In that case $\mathbf{q}(t)$ is an increasing function of time on the interval $[0, t_D^*]$, and for all $0 < t < t_D^*$ we have $1 < \mathbf{q}(t) < 1 + D$. Assume first that $t_D^* \leq T$. Under that circumstance, we have

$$\mathbf{q}(t_D^*) - \mathbf{q}(0) = D \leq \int_0^{t_D^*} f(u, \mathbf{q}(u)) du \leq 2\mathbf{s}_0 \tilde{C}(D + 1)t_D^*,$$

where we have used the upper bound (5.1) on f . As a consequence, we recover, still under the assumption $t_D^* \leq T$, the information

$$\begin{aligned} t_D^* &\geq \frac{D}{2\mathbf{s}_0 \tilde{C}(D + 1)} = \frac{(1 + \frac{1}{4\tilde{C}^2})^{\frac{1}{2}} - 1}{(1 + \frac{1}{4\tilde{C}^2})^{\frac{1}{2}}} \frac{1}{2\kappa h M_V^{(3)} \tilde{C}} \\ &\geq \left[\left(1 + \frac{1}{4\tilde{C}^2} \right)^{\frac{1}{2}} - 1 \right] \frac{1}{2\kappa h M_V^{(3)} \tilde{C}}, \end{aligned}$$

from which it follows

$$R > \frac{1}{16hM_V^{(3)}\kappa\tilde{C}^3}. \quad (5.3)$$

In the opposite situation where $t_D^* \geq T$, we anyhow recover, using (5.2)

$$R > T \geq \frac{1}{16hM_V^{(3)}\kappa\tilde{C}^2} \geq \frac{1}{16hM_V^{(3)}\kappa\tilde{C}^3},$$

where we have used that one may assume $\tilde{C} \geq 1$ without loss of generality. As a consequence of all these computations, we are now in position to conclude that in any circumstance we have

$$1 \leq \mathbf{q}(t) \leq D+1 \quad \text{whenever} \quad 0 \leq t \leq \frac{1}{16hM_V^{(3)}\kappa\tilde{C}^3} = r.$$

In particular, the function $t \mapsto \mathbf{q}(t)$ is increasing positive on $[0, r]$, and therefore, so is $t \mapsto \mathbf{q}'(t) = f(t, \mathbf{q}(t))$. Going further, we deduce that for all $t \in (-r, r)$ we have

$$\mathbf{q}'(t) \leq \frac{\kappa h M_V^{(3)} \tilde{C} (D+1)}{1 - \frac{1}{4} - \frac{1}{4}} \leq 2\kappa h M_V^{(3)} \tilde{C} (D+1) \leq \sqrt{5} \kappa h M_V^{(3)} \tilde{C},$$

since $D+1 \leq \frac{\sqrt{5}}{2}$. It follows that

$$\mathbf{q}(-r) = 1 - \int_{-r}^0 \mathbf{q}'(s) ds \geq 1 - r \sqrt{5} \kappa h M_V^{(3)} \tilde{C} > 0.8.$$

This proves the estimates on $\mathbf{q}(t)$. The estimates for $\mathbf{x}(t)$ and $\mathbf{s}(t)$ are then obtained straightforwardly. \blacksquare

Lemma 5.2 *There exists a positive constant C depending only on $\alpha \geq 1$ and $d \in \mathbb{N}^*$ such that*

$$\forall \delta > 0, \quad \sum_{p \in \mathbb{Z}^d \setminus \{0\}} e^{-\delta|p|^{1/\alpha}} \leq \frac{C}{\delta^{\alpha d+1}}$$

Proof. Note that for all $N > 0$,

$$\begin{aligned} \sum_{p \in \mathbb{Z}^d \setminus \{0\}} e^{-\delta|p|^{1/\alpha}} &\leq \sum_{p \in \mathbb{Z}^d \setminus \{0\}} \left(\underbrace{(\delta|p|^{1/\alpha})^N e^{-\delta|p|^{1/\alpha}}}_{\leq N^N e^{-N}} \right) (\delta|p|^{1/\alpha})^{-N} \\ &\leq \left(\frac{N}{e} \right)^N \sum_{p \in \mathbb{Z}^d \setminus \{0\}} (\delta|p|^{1/\alpha})^{-N}. \end{aligned}$$

Then, choose $N = \alpha d + 1$. \blacksquare

Corollary 5.3 *There exists a positive constant C depending only on $\alpha \geq 1$, $d \in \mathbb{N}^*$ and ρ_V such that*

$$\forall \delta \in (0; \rho_V), \quad \sum_{p \in \mathbb{Z}^d} e^{-\delta|p|^{1/\alpha}} \leq \frac{C}{\delta^{\alpha d+1}}$$

References

- [1] D. Bambusi, B. Grebert, *Birkhoff normal form for PDEs with tame modulus*, Duke Math. J. 135 (2006) 507–567.
- [2] C. Besse, B. Bidégaray, S. Descombes, *Order estimates in time of splitting methods for the nonlinear Schrödinger equation*, SIAM J. Numer. Anal. 40 (2002), no. 5, 26–40.
- [3] B. Cano, *Conserved quantities of some Hamiltonian wave equations after full discretization*, Numer. Math. 103 (2006) 197–223.
- [4] D. Cohen, E. Hairer, C. Lubich, *Long-time analysis of nonlinearly perturbed wave equations via modulated Fourier expansions*, Arch. Ration. Mech. Anal. 187 (2008) 341–368.
- [5] G. Dujardin, *Analyse de méthodes d'intégration en temps des équation de Schrödinger*, PhD thesis, University Rennes 1 (2008).
- [6] G. Dujardin, E. Faou, *Normal form and long time analysis of splitting schemes for the linear Schrödinger equation with small potential*, Numer. Math. 108 (2007) 223–262.
- [7] G. Dujardin, E. Faou, *Long time behavior of splitting methods applied to the linear Schrödinger equation*, C. R. Math. Acad. Sci. Paris 344 (2007) 89–92.
- [8] H. L. Eliasson, S. B. Kuksin, *KAM for non-linear Schrödinger equation*, Preprint (2006)
- [9] E. Hairer, C. Lubich, G. Wanner, *Geometric Numerical Integration. Structure-preserving Algorithms for Ordinary Differential Equations*. Springer, Berlin, 2002.
- [10] E. Hairer, S. P. Nørsett, G. Wanner, *Solving Ordinary Differential Equations I. Nonstiff Problems.*, Springer Series in Computational Mathematics 8, Berlin, 1993, 2nd edition.
- [11] C. Lubich *On splitting methods for the Schrödinger-Poisson and cubic non-linear Schrödinger equations* Math. Comp. 77 (2008), 2141–2153.
- [12] M. Oliver, M. West, C. Wulff, *Approximate momentum conservation for spatial semidiscretizations of semilinear wave equations*, Numer. Math. 97 (2004), 493–535.
- [13] B. Leimkuhler, S. Reich, *Simulating Hamiltonian dynamics*. Cambridge Monographs on Applied and Computational Mathematics, 14. Cambridge University Press, Cambridge, 2004.
- [14] T. Jahnke, C. Lubich, *Error bounds for exponential operator splittings*, BIT 40 (2000), 735–744.
- [15] Z. Shang *Resonant and Diophantine step sizes in computing invariant tori of Hamiltonian systems* Nonlinearity 13 (2000), 299–308.