Normal form and long time analysis of splitting schemes for the linear Schrödinger equation with small potential.

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December 4, 2007

Abstract

We consider the linear Schrödinger equation on a one dimensional torus and its time-discretization by splitting methods. Assuming a non-resonance condition on the stepsize and a small size of the potential, we show that the numerical dynamics can be reduced over exponentially long time to a collection of two dimensional symplectic systems for asymptotically large modes. For the numerical solution, this implies the long time conservation of the energies associated with the double eigenvalues of the free Schrödinger operator. The method is close to standard techniques used in finite dimensional perturbation theory, but extended here to infinite dimensional operators.

MSC numbers: 65P10, 37M15, 37K55

1 Introduction

In this paper, we consider the time-discretization of the linear Schrödinger equation by splitting methods and analyze the long time behavior of the corresponding "numerical" solution. Since no approximation in space is made, the problem is infinite dimensional, and the classical theory used in the case of ordinary differential equations cannot be applied. In particular, the long time behavior of the solution cannot be understood by the use of classical backward error analysis, see [7, 11]: In the finite dimensional case, a stability argument is invoked by assuming that the numerical solution lies in a compact set of the phase space over very long time. In infinite dimension, the corresponding assumption would require the *a priori* control of the regularity of the numerical solution over long time (see [3, 10] for the case of the non-linear wave equation).

In the case of splitting methods, exponential methods or standard methods for highly oscillatory equations, it is well known that for some values of the step-size resonances appear, making the a priori assumption of uniform conservation of regularity irrelevant. In this work, we consider one of the simplest possible situations: The case of a splitting method applied to the linear periodic Schrödinger equation with an analytic and *small* potential in one space dimension. Moreover, we will consider the splitting scheme as a multiplicative symplectic perturbation of the free linear Schrödinger propagator, and show the quasi-persistence of the conservation properties over exponentially long time with respect to the size of the potential.

Before going on, let us mention that another possible way to analyze these problems could be using modulated Fourier expansions: See [4] where the techniques used to analyze the exact solutions of non linear wave equations are clearly aimed at being applied to numerical analysis.

Let us consider the linear Schrödinger equation in one space dimension

$$i\frac{\partial\varphi}{\partial t}(x,t) = -\frac{\partial^2\varphi}{\partial x^2}(x,t) + V(x)\varphi(x,t), \quad \text{with} \quad \varphi(x,0) = \varphi^0(x), \tag{1.1}$$

where $\varphi(x,t)$ is the complex unknown wave function depending on the space variable $x \in \mathbb{T} := \mathbb{R}/2\pi\mathbb{Z}$ and the time $t \geq 0$. The potential V is a real function and the function φ^0 is the initial value of the wave function at $t = 0$. In the following, we write $\Delta = \partial_{xx}$ the Laplace operator in x so that the equation (1.1) reads

$$i\partial_t\varphi(t) = H\varphi(t), \quad \varphi(0) = \varphi^0, \quad \text{with} \quad H = -\Delta + V. \tag{1.2}$$

For a given time step $h > 0$, we consider the approximation scheme

$$\varphi(h) \simeq \exp(ih\Delta)\exp(-ihV)\varphi(0) \tag{1.3}$$

where by definition, $\exp(ih\Delta)\varphi$ is the solution $\psi(t)$ at the time $t = h$ of the equation

$$i\partial_t\psi(t) = -\Delta\psi(t), \quad \text{with} \quad \psi(0) = \varphi, \tag{1.4}$$

and similarly $\exp(-ihV)\varphi$ is the solution $\psi(t)$ at the time $t = h$ of the equation

$$i\partial_t\psi(t) = V\psi(t), \quad \text{with} \quad \psi(0) = \varphi. \tag{1.5}$$

If the potential is smooth enough, it can be shown that the approximation (1.3) is a first order approximation of the solution of (1.1), see [12] and [2] (where the non-linear case is studied). Moreover, notice that the propagator associated with (1.3) is L^2-unitary and so the scheme conserves the L^2-norm as the exact propagator associated with (1.1) does. Splitting schemes are widely used to approximate the solution of (1.1) (see e.g. [5, 9] and the references therein) as they are simple to compute using fast Fourier transform: The free Schrödinger part (1.4) can be computed easily in terms of Fourier coefficients, while the solution of (1.5) is treated as an ordinary differential equation on the corresponding grid. Notice also that the Lie splitting scheme (1.3) is conjugated to the Strang splitting so that the long time behavior of these two schemes are equivalent (see Remark 2.5 below).

In the finite dimensional case, the behavior of splitting methods for hamiltonian systems is now well understood, see for instance [7]. In particular, the use of the Baker-Campbell-Hausdorff formula shows that for a sufficiently small stepsize depending on the highest eigenvalue of the problem, there exists a modified hamiltonian for the propagator (1.3). The numerical flow can thus be interpreted as the exact solution of a hamiltonian system, at least for exponentially long time with respect to the stepsize. This result holds true for the linear and the non-linear case. When moreover the system is integrable, the techniques of classical perturbation theory apply, and it can be shown that the modified hamiltonian associated with a symplectic numerical method remains integrable, and that invariant tori persist over exponentially long time (see [7], Chapter X, and the classical references therein).

It is worth noticing that in infinite dimension, the persistence of invariant tori for hamiltonian PDEs is a very difficult problem even for the exact solutions, and many progresses have been made very recently. For the case of the non-linear Schrödinger equation, we refer to [1] and [6] for results in this direction.

In our case, though the initial equation is linear, the splitting propagator can be viewed as a non-linear function of the infinite dimensional operators $-\Delta$ and V, and we use techniques similar to the one used in classical perturbation theory to put the propagator (1.3) under a normal form that will give information on the long time behavior of its solution.

The idea is to consider for a fixed time step h the family of propagators

$$L(\lambda) = \exp(ih\Delta)\exp(-ih\lambda V), \quad \lambda \in \mathbb{R}, \tag{1.6}$$

and to assume that V is analytic. For $\lambda = 0$, we see that $L(0)$ is the free linear Schrödinger propagator. The corresponding solution can be written explicitly in terms of Fourier coefficients. The dynamics is periodic in time and there is no mixing between the different Fourier modes. The regularity of the initial value is preserved.

In the case of the splitting scheme (1.6) when the perturbation parameter λ is small enough we show that after a linear change of variable realized by a L^2-unitary operator satisfying exponential decay conditions on its coefficients, the propagator $L(\lambda)$ can be put under a normal form and written as an *almost X-shaped* L^2-unitary operator, up to exponentially small terms with respect to the small parameter λ. The coefficients of such an operator vanish, except possibly on the diagonal and the co-diagonal and for asymptotically large modes with respect to λ. This implies the existence of two-dimensional invariant spaces in the new variables, made of functions with zero Fourier coefficients except possibly at the indexes k and $-k$ for a given $k \in \mathbb{N}$. This result is valid for modes $k \leq \lambda^{-\sigma}$ where $\sigma > 0$ and for exponentially long time with respect to λ.

To show this result, we use the following non-resonance condition on the stepsize (see [7, 13]): there exist $\gamma > 0$ and $\nu > 1$ such that

$$\forall\, k \in \mathbb{Z}, \quad k \neq 0, \quad \left| \frac{1 - e^{ihk}}{h} \right| \geq \gamma |k|^{-\nu}. \tag{1.7}$$

It can be shown that for a given $h_0 > 0$ close to 0, the set of time steps $h \in (0, h_0)$ that do not satisfy (1.7) has a Lebesgue measure $\mathcal{O}(h_0^{r+1})$ for some $r > 1$ (see [7, 13]). The precise results are given in the next section.

Using this almost X-shaped representation, we can analyze the long time behavior of the numerical solution and show that the dynamics can be reduced to two dimensional linear symplectic systems mixing the two modes k and $-k$ for $k \leq \lambda^{-\sigma}$. This implies in particular the quasi-conservation of the regularity of the initial solution for these asymptotically large modes.

2 Statement of the results

In this section, we give a precise formulation of the result and its consequences for the long time behavior of the solution. We then give a sketch of proof and the major ingredients used in the recipe. We conclude this section by showing with numerical experiments the necessity of the non-resonance condition.

2.1 The results

For a function $\psi \in L^2(\mathbb{T})$, the associated Fourier coefficients, for $n \in \mathbb{Z}$, are given by the formula

$$\hat{\psi}_n = \frac{1}{2\pi} \int_{\mathbb{T}} e^{-inx} \psi(x) \mathrm{d}x.$$

In all this paper, we identify a function ψ and its Fourier coefficients on $\mathbb{T}$, this means that we write for all $n \in \mathbb{Z}$, ψ_n for $\hat{\psi}_n$ and identify the collection $(\psi_n)_{n\in\mathbb{Z}}$ with the function ψ itself. We denote by $\|\psi\| = (\sum_{n\in\mathbb{Z}} |\psi_n|^2)^{1/2}$ the L^2-norm on $\mathbb{T}$. We also identify operators acting on $L^2(\mathbb{T})$ with operators acting on $l^2(\mathbb{Z})$. Such an operator S can thus be characterized by its complex coefficients $(S_{ij})_{(i,j)\in\mathbb{Z}^2}$. If $\psi = (\psi_n)_{n\in\mathbb{Z}} \in \mathbb{C}^Z$, the product $\varphi = S\psi$ is defined by the sequence $\varphi = (\varphi_n)_{n\in\mathbb{Z}}$ of $\mathbb{C}^{\mathbb{Z}}$ with components $\varphi_n := \sum_{k\in\mathbb{Z}} S_{nk}\psi_k$, provided the summation makes sense. For example, the bounded operator defined as the multiplication by V acting on $L^2(\mathbb{T})$ is identified with the bounded operator (also denoted V) whose coefficients are given for all $(i,j) \in \mathbb{Z}^2$ by $V_{ij} = \hat{V}_{i-j}$.

For two operators A and B, the product AB is the operator whose coefficients are given formally by the definition

$$\forall\, (i,j) \in \mathbb{Z}^2, \quad (AB)_{ij} = \sum_{k\in\mathbb{Z}} A_{ik} B_{kj}. \tag{2.1}$$

For a given operator $S = (S_{ij})_{i,j\in\mathbb{Z}}$, we denote by S^* its adjoint with coefficients

$$\forall\, (i,j) \in \mathbb{Z}^2, \quad S^*_{ij} = \overline{S}_{ji}$$

where the bar denotes the complex conjugation. We say that S is symmetric if it satisfies $S = S^*$, and that S is L^2-unitary if it satisfies $S^*S = \mathrm{Id}$.

For an operator S and $\rho \in \mathbb{R}^+$, we define set

$$\|S\|_\rho = \sup_{k,\ell\in\mathbb{Z}} \left(e^{\rho|k-\ell|} |S_{k\ell}| \right) \tag{2.2}$$

and we define $\mathcal{A}_\rho$ as the space of S with finite analytic operator norm $\|S\|_\rho < \infty$. The space $\mathcal{S}_\rho$ denotes the subspace of symmetric operators of $\mathcal{A}_\rho$.

We define moreover the set of *X-shaped* operators $\mathcal{X}_\rho$ made of the elements of $X \in \mathcal{A}_\rho$ for which we have

$$X_{k\ell} \neq 0 \Longrightarrow |k| = |\ell|.$$

For functions ψ on $\mathbb{T}$, we define

$$\|\psi\|_\rho = \sup_{k\in\mathbb{Z}} \left(e^{\rho|k|} |\psi_k| \right)$$

for a given positive number ρ, and set

$$U_\rho := \{ \ \psi \mid \|\psi\|_\rho < \infty \ \}$$

the corresponding function space[1] of functions on $\mathbb{T}$ with finite analytic norm.

Hypothesis 2.1 *We assume that there exists a function $\mathcal{V}$ and $\rho_V > 0$ such that $\mathcal{V}$ is analytic on a complex domain containing the closure $\bar{\Omega}$ of $\mathbb{T} + i(-\rho_V, \rho_V)$ and such that for all $x \in \mathbb{T}$, $V(x) = \mathcal{V}(x) \in \mathbb{R}$. Therefore, if M_V denotes the maximum of the function $|\mathcal{V}|$ on $\bar{\Omega}$, then we have for all $n \geq 0$, $\|V^n\|_{\rho_V} \leq M_V^n$.*

For a given $K > 0$ we define the set of indexes

$$I_K = \{(k,\ell) \in \mathbb{Z}^2 \quad | \quad |k| \leq K \quad \text{or} \quad |\ell| \leq K\}. \tag{2.3}$$

We then set $\mathcal{X}_\rho^K$ the set of operators that are *almost X-shaped* in the sense where

$$X_{k\ell} \neq 0 \Longrightarrow \Big(|k| = |\ell| \quad \text{or} \quad (k,\ell) \notin I_K \Big)$$

The aim of this paper is to prove the following conjugation result for the propagator:

Theorem 2.2 *Assume that V satisfies Hypothesis 2.1 and let $L(\lambda)$ be defined by (1.6). Assume $\gamma > 0$ and $\nu > 1$ are given. There exist positive constants λ_0, σ and c depending only on V, ρ_V, γ and ν, such that for all stepsize $h \in$*

[1] The notation $\|\cdot\|_\rho$ is not ambiguous: If an operator W is induced by a function, i.e. if $W_{ij} = \hat{\psi}_{i-j}$ for $(i,j) \in \mathbb{Z}^2$ and for a function ψ with Fourier coefficients $\hat{\psi}_n$, $n \in \mathbb{Z}$, then we have $\|W\|_\rho = \|\psi\|_\rho$.

$(0,1)$ *satisfying* (1.7), *there exist families of* L^2*-unitary operators* $Q(\lambda)$ *and* $\Sigma(\lambda)$ *analytic in* λ *for* $|\lambda| < \lambda_0$ *such that for* $\lambda \in (0, \lambda_0)$,

$$Q(\lambda) \in \mathcal{A}_{\rho_V/4} \quad \textit{and} \quad \Sigma(\lambda) \in \mathcal{X}^K_{\rho_V/4} \quad \textit{with} \quad K = \lambda^{-\sigma} \tag{2.4}$$

where $\sigma = 1/(32(\nu + 1)) > 0$,

$$\|Q(\lambda) - \mathrm{Id}\|_{\rho_V/4} \le \lambda^{1/2} \quad \textit{and} \quad \|\Sigma(\lambda) - e^{ih\Delta}\|_{\rho_V/4} \le h\lambda^{1/2}, \tag{2.5}$$

such that the following equality holds:

$$Q(\lambda)L(\lambda)Q(\lambda)^* = \Sigma(\lambda) + R(\lambda). \tag{2.6}$$

Moreover, the remainder term $R(\lambda)$ *satisfies, for* $\lambda \in (0, \lambda_0)$,

$$\|R(\lambda)\|_{\rho_V/5} \le \exp(-c\lambda^{-\sigma}). \tag{2.7}$$

Roughly speaking, the preceding result shows that after a unitary change of variables close to the identity in some analytic operator norm, the dynamics can be reduced, up to exponentially small terms, to the action of $\Sigma(\lambda)$ which decouples into 2×2 symplectic systems for each modes $\pm k$. This is valid for asymptotically large modes $|k| \le \lambda^{-\sigma}$. More precisely, if φ is a function and if $\psi = \Sigma(\lambda)\varphi$, we have for $|k| \le \lambda^{-\sigma}$,

$$\begin{pmatrix} \psi_k \\ \psi_{-k} \end{pmatrix} = \begin{pmatrix} a_k(\lambda) & b_k(\lambda) \\ c_k(\lambda) & d_k(\lambda) \end{pmatrix} \begin{pmatrix} \varphi_k \\ \varphi_{-k} \end{pmatrix} \tag{2.8}$$

where the 2×2 matrix in this equality is close to the diagonal matrix with entries e^{-ihk^2}, and is unitary. This implies that we have for all k such that $|k| \le \lambda^{-\sigma}$,

$$|\psi_k|^2 + |\psi_{-k}|^2 = |\varphi_k|^2 + |\varphi_{-k}|^2. \tag{2.9}$$

Combining the conservation law (2.9) of $\Sigma(\lambda)$ with the exponential estimate (2.7) will allow us to derive long time bounds for the iterates of $L(\lambda)$.

In the following, for a function φ, we use the notation

$$|\varphi|_0^2 = |\varphi_0|^2 \quad \text{and} \quad \forall\, k \in \mathbb{Z}\backslash\{0\}, \quad |\varphi|_k^2 = |\varphi_k|^2 + |\varphi_{-k}|^2 \tag{2.10}$$

to denote the energies at the frequency $|k|$.

Moreover, for $s > 0$ we introduce the norm[2]

$$\|\varphi\|_{s,\infty} = \sup_{k \ge 0} \left((1 + k)^s |\varphi|_k\right). \tag{2.11}$$

Using the preceding remark and the estimates on the remainder term, we can show the following corollary, which yields long time results for the approximated solution:

[2]Note that $\|\varphi\|_{s,\infty} < \infty$ implies that φ is in the Sobolev space $H^{s-1/2-\varepsilon}$ for all $\varepsilon > 0$. If for instance $\|\varphi\|_{s,\infty} < \infty$ for some $s > 1/2$ then $\varphi \in L^2$.

Corollary 2.3 *We use the notations of the previous Theorem. For $n \in \mathbb{N}$, we set $\varphi^n = L(\lambda)^n \varphi^0$.*

(i) *There exists a constant $C > 0$ depending only on V, ρ_V, γ and ν such that for all $h \in (0,1)$ satisfying* (1.7)*, all $\lambda \in (0, \lambda_0)$, $n \le \exp(c\lambda^{-\sigma}/2)$, and $\varphi^0 \in L^2(\mathbb{T})$,*

$$\forall\, k \in \mathbb{N}, \quad k \le \lambda^{-\sigma}, \quad \big|\, |\varphi^n|_k - |\varphi^0|_k \,\big| \le C\lambda^{1/2} \|\varphi^0\| \,. \tag{2.12}$$

(ii) *Assume that $s > 1/2$ is given, and let s' be such that $s - s' \ge 1/2$. Then there exists a constant c_s depending only on V, ρ_V, γ, ν and s, such that for all $h \in (0,1)$ satisfying* (1.7)*, all $\lambda \in (0, \lambda_0)$, $n \le \exp(c\lambda^{-\sigma}/2)$, and φ^0 such that $\|\varphi^0\|_{s,\infty} < +\infty$, we have*

$$\sup_{0 \le k \le \lambda^{-\sigma}} \Big((1+k)^{s'} \,\big|\, |\varphi^n|_k - |\varphi^0|_k \,\big| \Big) \le c_s \lambda^{1/2} \|\varphi^0\|_{s,\infty} . \tag{2.13}$$

(iii) *For all $\rho \in (0, \rho_V/5)$, there exist positive constants μ_0 and C (depending only on V, ρ_V, γ, ν and ρ) such that for all $h \in (0,1)$ satisfying* (1.7)*, all $\lambda \in (0, \lambda_0)$, $n \le \exp(c\lambda^{-\sigma}/2)$, $\mu \in (0, \mu_0)$ and $\varphi^0 \in U_\rho$,*

$$\sup_{0 \le k \le \lambda^{-\sigma}} \Big(e^{\mu k} \,\big|\, |\varphi^n|_k - |\varphi^0|_k \,\big| \Big) \le C \lambda^{1/2} \|\varphi^0\|_{\rho} . \tag{2.14}$$

Remark 2.4 We could also diagonalize the 2×2 matrix in (2.8). As the eigenvalues are close to e^{ihk^2}, we could obtain this way a quasiperiodic behavior of the numerical solution in suitable coordinates, with frequencies of the form $k^2 + \mathcal{O}(\lambda^{1/2})$. However, as e^{ihk^2} is a double eigenvalue of the limit matrix, this would not imply the continuity of the transformation in terms of the small parameter λ. ■

Remark 2.5 The same results hold true for the family of Strang splitting propagators

$$\exp(ih\Delta/2)\exp(-ih\lambda V)\exp(ih\Delta/2)$$

which are conjugated to the Lie splitting schemes (1.6) by the operator $\exp(ih\Delta/2)$ that defines an isometry between all $\mathcal{A}_\rho$ spaces. ■

Remark 2.6 The choice of $\rho_V/4$ and $\rho_V/5$ in Theorem 2.2 is made for convenience in the proof, and could be replaced by any number of the type $\rho_V - \delta$ with $0 < \delta < \rho_V$. This would only change the values of the constants in the statements. ■

2.2 Sketch of proof

The proof of Theorem 2.2 is divided into several steps. We describe here the main arguments:

(i) Operator formal series. We first seek the operators $Q(\lambda)$ and $\Sigma(\lambda)$ as formal series of the form

$$Q(\lambda) = \sum_{n \geq 0} \lambda^n Q_n \quad \text{and} \quad \Sigma(\lambda) = \sum_{n \geq 0} \lambda^n \Sigma_n$$

where for all $n \in \mathbb{N}$, the coefficients of the operators Q_n and Σ_n satisfy exponential decay conditions of the form (2.2) and where the equation

$$Q(\lambda)L(\lambda)Q(\lambda)^* = \Sigma(\lambda) \tag{2.15}$$

is satisfied in the sense of formal series. Note that as V is a bounded operator, the formal series $L(\lambda)$ is in fact a power series in λ.

In order to ensure the fact that $Q(\lambda)$ and $\Sigma(\lambda)$ are unitary operators, we introduce the "logarithm" formal series

$$S = Q^*(i\partial_\lambda Q) \quad \text{and} \quad X = \Sigma^*(i\partial_\lambda \Sigma)$$

and we look for symmetric coefficients in the formal series $S(\lambda)$ and $X(\lambda)$. Writing down the equations for the coefficients, we see that for all $n \geq 0$, S_n and X_n have to satisfy an equation that reads

$$S_n - e^{ih\Delta} S_n e^{-ih\Delta} + X_n = G_n \tag{2.16}$$

where G_n is symmetric and depends on V, S_p and X_p for $p = 0, \ldots, n-1$. The study of the homological equation (2.16) is thus the cornerstone for the recursive construction of the operators. The goal of the first part of Section 3 is to make explicit the recursive equalities (2.16).

(ii) Solution of the homological equation. In the second part of Section 3, we consider the equation

$$S - e^{-ih\Delta} S e^{ih\Delta} + X = G$$

where G is a given symmetric operator. In terms of coefficients, as the Laplace operator is a diagonal operator with entries $-k^2$, $k \in \mathbb{Z}$, this equation can be written

$$(1 - e^{ih(k^2 - \ell^2)}) S_{k\ell} + X_{k\ell} = G_{k\ell}$$

for $(k, \ell) \in \mathbb{Z}^2$. We see that in the case where $k^2 = \ell^2$, the value of $X_{k\ell}$ is imposed. This is the reason for the definition of X-shaped operators. Moreover, a problem of small divisors may appear when $h(k^2 - \ell^2)$ is close to a multiple of 2π. The use of the condition (1.7) allows in principle to determine a solution

$$S_{k\ell} = \frac{1}{1 - e^{ih(k^2 - \ell^2)}} G_{k\ell}$$

for $k^2 \neq \ell^2$. However, the condition (1.7) and the previous equality do not imply that S is in a space of exponentially decaying matrices $\mathcal{A}_\rho$ for a suitable ρ if G is. This is due to possibly unbounded coefficients $k + \ell$ in the term $|k^2 - \ell^2|$.

This is the reason for the introduction of the set of indexes I_K in (2.3) and the corresponding I_K-solution of the homological equation (see Definition 3.1 below). This explains the final form of the propagator $\Sigma(\lambda)$.

Thanks to the non-resonance condition (1.7), we are now able to state a result for the I_K-solutions of the recursive homological equations, see Proposition 3.2. In particular, we obtain the estimates (3.18) which are familiar in backward error analysis and in classical perturbation theory.

(iii) Estimates and optimization of the constants. Sections 4 and 5 are the most technical ones and show the precise estimates of the Theorem. Using I_K-solutions of the recursive homological equations, we can prove analytic estimates for the coefficients S_n and X_n: see Proposition 4.1. We obtain that for large n, the analytical norms of these coefficients are bounded by

$$(K^\alpha n^\beta)^n$$

up to some constants, and for suitable positive coefficients α and β. Though these series diverge, we can define for a fixed index N, the corresponding truncated series and operators $Q^{[N]}(\lambda)$ and $\Sigma^{[N]}(\lambda)$ that satisfy the equation (2.15) up to a remainder term $R^{[N]}(\lambda)$ depending on N. We then use these estimates to give a bound for the remainder term, see Proposition 5.3. Roughly speaking, the remainder term is bounded in a suitable $\mathcal{A}_\rho$ space by

$$(\lambda K^\alpha N^\beta)^N$$

for $\lambda \in (0, \lambda_0)$ and up to some constant. We then take K and N proportional to a negative power of λ to obtain an exponential estimate of the form (2.7).

(iv) Proof of Corollary 2.3. Section 6 is devoted to the proof of this corollary. The idea is to use the almost X-shaped form of $\Sigma(\lambda)$ and the estimate (2.7) of the remainder term $R(\lambda)$. We divide the phase space into the spaces $\{\varphi \,|\, \varphi_k = 0, \quad |k| \leq K\}$ and $\{\varphi \,|\, \varphi_k = 0, \quad |k| > K\}$. If π_K denotes the L^2-orthogonal projection onto the latter space, the almost X-shaped structure of $\Sigma(\lambda)$ implies that $[\Sigma(\lambda), \pi_K] = 0$ so that these spaces are invariant by $\Sigma(\lambda)$. The ingredients to show the results are the following two key estimates: If for all $n \in \mathbb{N}$, we set $\psi^n = Q(\lambda)\varphi^n$, then we prove that for $n \leq \exp(c\lambda^{-\sigma}/2)$ we have

$$\forall\, 0 \leq k \leq K, \quad \big|\, |\psi^n|_k - |\psi^0|_k \big| \leq C \exp(-c\lambda^{-\sigma}/2) \|\varphi^0\|$$

for a constant C depending only on V, ρ_V and the parameters appearing in the non-resonance condition (1.7) . This shows the extremely good conservation of the energies at a given mode $k \leq K = \lambda^{-\sigma}$ in the "new" variables, and yields easily the estimates of the corollary for ψ^n. In order to get back to the original variables, we have to control the modes with indexes greater than K by showing that for $n \leq \exp(c\lambda^{-\sigma}/2)$,

$$\Big| \|\pi_K \psi^n\| - \|\pi_K \psi^0\| \Big| \leq C \exp(-c\lambda^{-\sigma}/2) \|\varphi^0\|$$

where C does not depend on λ. The results are obtained by combining these two estimates, and by using the fact that for a smooth function, the term $\|\pi_K \psi^0\|$ is small for big $K = \lambda^{-\sigma}$.

2.3 Numerical experiments

We consider the case where the potential function and the initial wave function are given by

$$V(x) = \frac{3}{5 - 4\cos(x)} \quad \text{and} \quad \varphi^0(x) = \frac{2}{2 - \cos(x)}.$$

We use two different time steps:

$$h = 0.2 \quad \text{and} \quad h = \frac{2\pi}{6^2 - 2^2} = 0.196\ldots. \tag{2.17}$$

The first time step satisfies the non-resonance condition[3] (1.7) while the second one is obviously resonant. We use fast Fourier transformations to compute the solution of (1.3). In Figure 1, we take $2^7 + 1 = 129$ Fourier modes. We make 10^6 iterations, and we set $\lambda = 0.1$. We plot the first 5 energies $|\varphi^n|_k$, $k = 0, \ldots, 4$ in logarithmic scale. We see that if the non-resonance condition is not satisfied, the conservation properties are lost.

In Figure 2, we use $2^9 + 1 = 513$ Fourier modes and plot all the energies for 10^5 iterations with $\lambda = 0.01$. We see the growth of high order modes (recall that the L^2-norm is conserved).

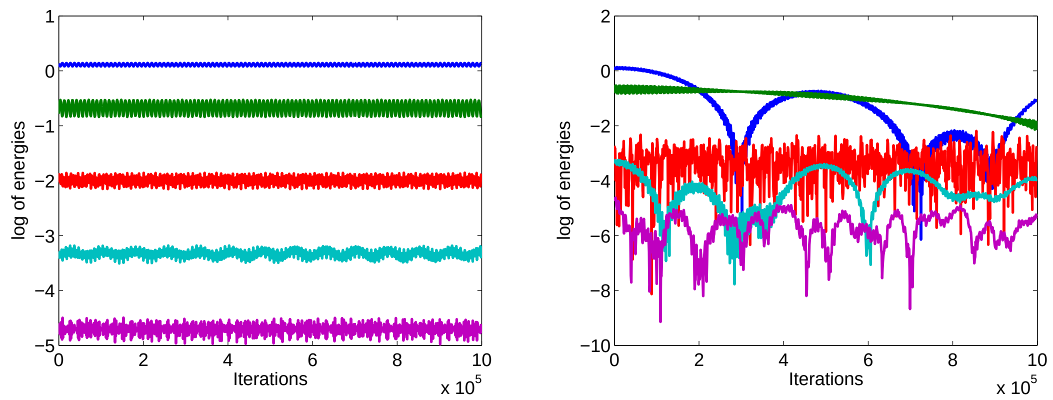

Figure 1: Energies of the 5 first modes in logarithmic scale, $\lambda = 0.1$. Non-resonant stepsize (left) and resonant stepsize (right)

3 Formal series and homological equation

3.1 Operator formal series

We now start the proof of Theorem 2.2. In this Section, we consider all the operators as formal series operators in λ. We show rigorous estimates in the

[3] We thank Z. Shang who showed us this fact.

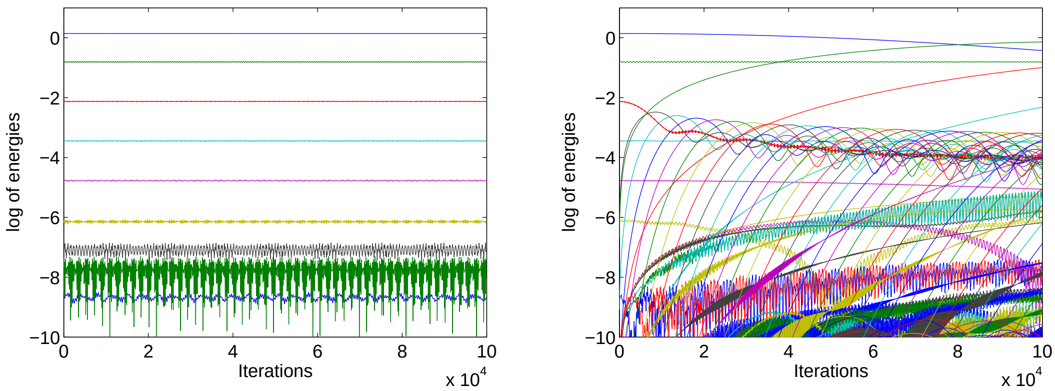

Figure 2: Energies in logarithmic scale, $\lambda = 0.01$. Non-resonant stepsize (left) and resonant stepsize (right)

next section. Let $A(\lambda) = \sum_{n\geq 0} \lambda^n A_n$ and $B(\lambda) = \sum_{n\geq 0} \lambda^n B_n$ be two formal series whose coefficients respectively are operators A_n and B_n. The product $A(\lambda)B(\lambda) = C(\lambda)$ is the formal series $C(\lambda) = \sum_{n\geq 0} \lambda^n C_n$ with coefficients

$$C_n = \sum_{k=0}^{n} A_k B_{n-k}, \quad n \geq 0,$$

where the product between A_k and B_{n-k} is the operator product defined in (2.1). Similarly, we can define the action of the derivative in λ on formal series by

$$\partial_\lambda A(\lambda) = \sum_{n\geq 0} \lambda^n (n+1) A_{n+1}$$

for a formal series $A(\lambda) = \sum_{n\geq 0} \lambda^n A_n$.

Recall that $L(\lambda)$ is given by (1.6). As a formal series in λ, we write

$$L(\lambda) = \sum_{n\geq 0} \frac{\lambda^n}{n!} e^{ih\Delta}(-ihV)^n.$$

We thus have the equalities

$$i\partial_\lambda L(\lambda) = e^{ih\Delta} hV e^{-ih\Delta} L(\lambda) \qquad \text{and} \qquad L(0) = e^{ih\Delta}.$$

We now seek formal series $Q(\lambda) = \sum_{n\geq 0} \lambda^n Q_n$ and $\Sigma(\lambda) = \sum_{n\geq 0} \lambda^n \Sigma_n$ satisfying

$$Q(\lambda) L(\lambda) Q(\lambda)^* = \Sigma(\lambda), \tag{3.1}$$

such that

$$Q(\lambda)^* Q(\lambda) = \mathrm{Id} \quad \text{and} \quad \Sigma(\lambda)^* \Sigma(\lambda) = \mathrm{Id}, \tag{3.2}$$

and where $\Sigma(\lambda)$ is an X-shaped operator.

Taking the derivative $i\partial_\lambda$ of the equation (3.1) yields

$$(i\partial_\lambda Q)LQ^* - QL(i\partial_\lambda Q)^* + hQe^{ih\Delta}Ve^{-ih\Delta}LQ^* = i\partial_\lambda \Sigma,$$

whence

$$Q^*(i\partial_\lambda Q)L - L(i\partial_\lambda Q)^*Q + he^{ih\Delta}Ve^{-ih\Delta}L = Q^*(i\partial_\lambda \Sigma)Q. \tag{3.3}$$

We introduce the operators

$$S = Q^*(i\partial_\lambda Q) \quad \text{and} \quad X = \Sigma^*(i\partial_\lambda \Sigma).$$

The formal series Q and Σ can be reconstructed from the series S and X using the initial conditions $Q(0) = \mathrm{Id}$ and $\Sigma(0) = e^{ih\Delta}$.

Note that if the formal series S and X are symmetric, Q and Σ are unitary (i.e. satisfy (3.2)). Moreover, if X an X-shaped operator, Σ will also be X-shaped.

Assuming S is symmetric, the equation (3.3) can be written (we use $\Sigma = QLQ^*$)

$$SL - LS + he^{ih\Delta}Ve^{-ih\Delta}L = Q^*\Sigma XQ = LQ^*XQ$$

whence, as V and $e^{-ih\lambda V}$ commute, and as $L^*L = \mathrm{Id}$,

$$S - L^*SL = hV - Q^*XQ. \tag{3.4}$$

Our formal series problem will hence be the following: Find formal series $S(\lambda) = \sum_{n\geq 0} \lambda^n S_n$ and $X(\lambda) = \sum_{n\geq 0} \lambda^n X_n$ such that for all $n \geq 0$, $S_n^* = S_n$, $X_n^* = X_n$ and X_n is a X-shaped operator, satisfying the equation

$$S(\lambda) - L^*(\lambda)S(\lambda)L(\lambda) = hV - Q^*(\lambda)X(\lambda)Q(\lambda) \tag{3.5}$$

where the operator Q satisfies

$$i\partial_\lambda Q(\lambda) = Q(\lambda)S(\lambda), \quad \text{and} \quad Q(0) = \mathrm{Id}. \tag{3.6}$$

The operator Σ will then be reconstructed using the formulae

$$i\partial_\lambda \Sigma(\lambda) = \Sigma(\lambda)X(\lambda), \quad \text{and} \quad \Sigma(0) = e^{ih\Delta}. \tag{3.7}$$

3.2 Coefficients

We now write the previous formal series equations in terms of the coefficients of the operator formal series. The equation (3.6) can be written: For all $n \geq 0$,

$$i(n+1)Q_{n+1} = \sum_{k=0}^{n} Q_k S_{n-k}. \tag{3.8}$$

The equation (3.7) yields similar equalities for Σ_n and X_n. Note that we impose $Q_0 = I$ and $\Sigma_0 = e^{ih\Delta}$.

Let us write the coefficients of the equation (3.5): For all $n \in \mathbb{N}$,

$$S_n - \sum_{p+q+r=n} \frac{(ihV)^p}{p!} e^{-ih\Delta} S_q e^{ih\Delta} \frac{(-ihV)^r}{r!} = \delta_n^0 hV - \sum_{p+q+r=n} Q_p^* X_q Q_r. \quad (3.9)$$

Assuming that S_k and X_k are determined for $k = 0, \cdots, n-1$ and that they are symmetric, the equation (3.9) can be written

$$S_n - e^{-ih\Delta} S_n e^{ih\Delta} + X_n = \delta_n^0 hV$$
$$+ \sum_{\{p+q+r=n | q \neq n\}} \left(\frac{(ihV)^p}{p!} e^{-ih\Delta} S_q e^{ih\Delta} \frac{(-ihV)^r}{r!} - Q_p^* X_q Q_r \right). \quad (3.10)$$

Since the summation set is symmetric in r and p, the right hand side of this equation is symmetric.

We thus see that for all n, we have to solve a homological equation

$$S_n - e^{-ih\Delta} S_n e^{ih\Delta} + X_n = G_n, \quad (3.11)$$

where G_n is symmetric, and where we seek S_n and X_n symmetric with X_n a X-shaped operator.

Let us first consider the equation (3.10) for $n = 0$. We have

$$S_0 - e^{-ih\Delta} S_0 e^{ih\Delta} + X_0 = hV. \quad (3.12)$$

The operator Δ is diagonal with entries $-k^2$, $k \in \mathbb{Z}$. Hence for $(k, \ell) \in \mathbb{Z}^2$, the previous equation can be written

$$(S_0)_{k\ell}(1 - e^{ih(k^2 - \ell^2)}) = hV_{k\ell} - (X_0)_{k\ell}$$

so that we can choose for $k^2 \neq \ell^2$, under the condition that $h(k^2 - \ell^2)$ is not a multiple of 2π,

$$(S_0)_{k\ell} = \frac{1}{1 - e^{ih(k^2 - \ell^2)}} hV_{k\ell} \quad \text{and} \quad (X_0)_{k\ell} = 0 \quad (3.13)$$

so that X_0 is X-shaped. For $k^2 = \ell^2$ the previous equation degenerates, but we can take

$$(S_0)_{k\ell} = 0 \quad \text{and} \quad (X_0)_{k\ell} = hV_{k\ell}.$$

The previous equations define symmetric operators S_0 and X_0, and X_0 is X-shaped. By induction, the formal series problem of the previous subsection is then solved. However, we cannot obtain estimates in $\mathcal{A}_\rho$-spaces for the operators, even if h satisfies the estimate (1.7). The reason for this is that using (1.7), the equation (3.13) yields the following estimate, for $k \neq \ell$,

$$|(S_0)_{k\ell}| \leq \gamma^{-1} |k^2 - \ell^2|^\nu |V_{k\ell}|$$

and the fact that $V \in \mathcal{A}_{\rho_V}$ does not implies that $S_0 \in \mathcal{A}_\rho$ for a suitable ρ. This is due to the possibly unbounded coefficients $k + \ell$.

3.3 Solution of the homological equation

It is worth noticing that the above equation (3.11) is underdetermined. The previous computations motivate the introduction of the following solutions of the homological equation:

Definition 3.1 Let G be a symmetric operator and $K > 0$ be a real number. Assume that $h \in (0,1)$ satisfies (1.7). Let us consider the equation:

$$S - e^{ih\Delta} S e^{-ih\Delta} + X = G. \tag{3.14}$$

We define as I_K-solution of the homological equation (3.14) the symmetric operators S and X defined for $(k,l) \in \mathbb{Z}^2$ by

$$\text{if } (k,\ell) \in I_K \text{ and } |k| \neq |\ell|, \quad \begin{cases} S_{k\ell} &= \dfrac{1}{1 - e^{ih(k^2-\ell^2)}} G_{k\ell}, \\ X_{k\ell} &= 0, \end{cases} \tag{3.15}$$

$$\text{otherwise, if } (k,\ell) \notin I_K \text{ or } |k| = |\ell|, \begin{cases} S_{k\ell} &= 0, \\ X_{k\ell} &= G_{k\ell}, \end{cases} \tag{3.16}$$

where I_K is defined in (2.3). ■

With this definition, the following theorem yields the cornerstone of the solving process:

Proposition 3.2 *Let $G \in \mathcal{S}_\rho$ for a given $\rho > 0$. Assume that h satisfies* (1.7) *with the constants γ and ν. Let S and X be the I_K-solutions of the homological equation*

$$S - e^{-ih\Delta} S e^{ih\Delta} + X = G \tag{3.17}$$

for a given $K \geq 1$. Then for all δ such that $0 < \delta \leq \rho$, we have $S \in \mathcal{S}_{\rho-\delta}$, $X \in \mathcal{S}_\rho \cap \mathcal{X}_\rho^K$, and the following estimates hold:

$$\|S\|_{\rho-\delta} \leq \frac{K^\nu}{\gamma h} \left(\frac{4\nu}{e\delta} \right)^{2\nu} \|G\|_\rho \quad \textit{and} \quad \|X\|_\rho \leq \|G\|_\rho . \tag{3.18}$$

Proof. The fact that $\|X\|_\rho \leq \|G\|_\rho$ is clear from (3.16).
Using (3.15) and (1.7), we have for $(k,\ell) \in I_K$ and $|k| \neq |\ell|$,

$$|S_{k\ell}| \leq \frac{1}{\gamma h} |k^2 - \ell^2|^\nu |G_{k\ell}|.$$

But for $(k,\ell) \in I_K$, we easily see that $|k + \ell| \leq 2K + |k - \ell|$. Hence we have

$$\begin{aligned} |k^2 - \ell^2|^2 &\leq |k-\ell|^2 (2K + |k-\ell|)^2 \\ &\leq 2|k-\ell|^2 (4K^2 + |k-\ell|^2) \\ &\leq 8K^2 |k-\ell|^2 + 2|k-\ell|^4 \\ &\leq 16K^2 |k-\ell|^4 \end{aligned}$$

and therefore $|k^2 - \ell^2|^\nu \le 2^{2\nu} K^\nu |k-\ell|^{2\nu}$. This implies that for all $(k,\ell) \in I_K$ with $|k| \ne |\ell|$,

$$|S_{k\ell}| \le \frac{K^\nu}{\gamma h} 2^{2\nu} |k-\ell|^{2\nu} \|G\|_\rho \, e^{-\rho|k-\ell|}.$$

Hence, for all $(k,\ell) \in \mathbb{Z}^2$,

$$|S_{k\ell}| e^{(\rho-\delta)|k-\ell|} \le \frac{K^\nu}{\gamma h} 2^{2\nu} \|G\|_\rho \, |k-\ell|^{2\nu} e^{-\delta|k-\ell|}.$$

The fact that for all $(k,\ell) \in \mathbb{Z}^2$,

$$|k-\ell|^{2\nu} e^{-\delta|k-\ell|} \le \left(\frac{2\nu}{e\delta}\right)^{2\nu}$$

allows to conclude. ∎

In the next section, we will consider the recursive solutions of the collection of equations (3.10) by induction on n using the I_K-solutions of the homological equation and the previous Proposition.

4 Estimates for the coefficients

We now give estimates for the coefficients of the formal series $S(\lambda)$, $X(\lambda)$ and $Q(\lambda)$ given by the recursive I_K-solutions of (3.10) for a fixed $K \ge 1$. Recall that V is assumed to satisfy Hypothesis 2.1.

Let us first consider the operators S_0 and X_0 given by the I_K-solution of (3.12). Using Proposition 3.2, we have for all $0 < \delta \le \rho_V$

$$\|S_0\|_{\rho_V - \delta} \le M_V \frac{K^\nu}{\gamma} \left(\frac{4\nu}{e\delta}\right)^{2\nu} \quad \text{and} \quad \|X_0\|_{\rho_V} \le h M_V. \tag{4.1}$$

In particular, there exists a constant C depending only on V, ρ_V, γ and ν such that

$$\|S_0\|_{\rho_V/3} \le K^\nu C \quad \text{and} \quad \|X_0\|_{\rho_V/3} \le hC. \tag{4.2}$$

Moreover, since $Q_0 = \mathrm{Id}$, we have that $\|Q_0\|_{\rho_V/3} = 1$.

The goal of this section is to prove the following result:

Proposition 4.1 *There exist constants $C_0 \ge 1$ and $K_0 \ge 1$ depending only on V, ρ_V, γ and ν such that for all $K \ge K_0$, and all $h \in (0,1)$ satisfying* (1.7)*, if we denote by $(S_J)_{J\ge 0}$, $(Q_J)_{J \ge 0}$ and $(X_J)_{J\ge0}$ the operators obtained by the iterative I_K-solutions of* (3.10)*, we have for all $J \ge 1$,*

$$\|S_J\|_{\rho_V/3} + \|Q_J\|_{\rho_V/3} \le \left(C_0 K^\alpha J^\beta\right)^J \quad \textit{and} \tag{4.3}$$

$$\|X_J\|_{\rho_V/3} \le h\left(C_0 K^\alpha J^\beta\right)^J, \tag{4.4}$$

where $\alpha = 2\nu$ and $\beta = 4\nu + 3$.

Before giving the proof of this proposition, we first give the following lemma that provides a bound for the product of two operators with exponential decay of coefficients away from the diagonal:

Lemma 4.2 *Let $\rho \geq 0$ and $\delta > 0$. Let $A \in \mathcal{A}_\rho$ and $B \in \mathcal{A}_{\rho+\delta}$. Then the products AB and BA are in the space $\mathcal{A}_\rho$ and we have the estimates*

$$\|AB\|_\rho \leq C_\delta \, \|A\|_\rho \, \|B\|_{\rho+\delta} \quad \textit{and} \quad \|BA\|_\rho \leq C_\delta \, \|A\|_\rho \, \|B\|_{\rho+\delta}\,, \tag{4.5}$$

where $C_\delta = (1+e^{-\delta})(1-e^{-\delta})^{-1} > 1$.

Proof. By definition, we have for $(k,\ell,m) \in \mathbb{Z}^3$

$$|A_{k\ell}| \leq \|A\|_\rho \, e^{-\rho|k-\ell|} \quad \text{and} \quad |B_{\ell m}| \leq \|B\|_{\rho+\delta} \, e^{-(\rho+\delta)|\ell-m|}. \tag{4.6}$$

This implies that for all $(k,m) \in \mathbb{Z}^2$,

$$|(AB)_{km}| e^{\rho|k-m|} \leq \|A\|_\rho \, \|B\|_{\rho+\delta} \, e^{\rho|k-m|} \sum_{\ell \in \mathbb{Z}} e^{-\rho|k-\ell|} e^{-(\rho+\delta)|\ell-m|}.$$

The last sum can also be written after the change of index $\ell \mapsto \ell + m$,

$$\sum_{\ell\in\mathbb{Z}} e^{-\rho|k-\ell-m|} e^{-\rho|\ell|} e^{-\delta|\ell|} \leq \sum_{\ell\in\mathbb{Z}} e^{-\rho|k-m|} e^{+\rho|\ell|} e^{-\rho|\ell|} e^{-\delta|\ell|}$$

where we used $|k-m| - |\ell| \leq |k-m-\ell|$ for all $(k,m,\ell) \in \mathbb{Z}^3$. We thus have

$$\|AB\|_\rho \leq \|A\|_\rho \, \|B\|_{\rho+\delta} \sum_{\ell\in\mathbb{Z}} e^{-\delta|\ell|}$$

and we easily compute that

$$\sum_{\ell\in\mathbb{Z}} e^{-\delta|\ell|} = \frac{1+e^{-\delta}}{1-e^{-\delta}} \tag{4.7}$$

which yields the first inequality in (4.5). The second is proved similarly. ∎

Proof of Proposition 4.1. Let $J \geq 1$ be a fixed integer. We set $\delta = \rho_V(2J+1)^{-1}$ and for $j \in \{0,\dots,J+1\}$, $\rho_j = \rho_V - j\delta = (2J+1-j)\delta$.
In the following, for all operator A and for $j \in \{0,\dots,J+1\}$, we set

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

Note that if $0 \leq j \leq k \leq J+1$, then $\|A\|_{(k)} \leq \|A\|_{(j)}$. Moreover, $\|A\|_{(0)} = \|A\|_{\rho_V}$ and $\|A\|_{(J+1)} = \|A\|_{\rho_V J/(2J+1)} \geq \|A\|_{\rho_V/3}$.
The inequalities (4.1) and the fact that $Q_0 = \mathrm{Id}$ yield with the previous notations:

$$\|S_0\|_{(1)} \leq M_V \frac{K^\nu}{\gamma} \Big(\frac{4\nu}{e\delta}\Big)^{2\nu}, \quad \|X_0\|_{(0)} \leq hM_V \quad \text{and} \quad \|Q_0\|_{(0)} = 1.$$

We now seek recursive bounds for the norms $\|S_j\|_{(j+1)}$, $\|X_j\|_{(j)}$ and $\|Q_j\|_{(j)}$ for $j = 0,\dots,J$.

The equality (3.8) and Lemma 4.2 ensure that, for $n = 0, \dots, J-1$, we have

$$(n+1)\|Q_{n+1}\|_{(n+1)} \le \sum_{k=0}^{n} \|Q_k S_{n-k}\|_{(n+1)} \le C_\delta \sum_{k=0}^{n} \|Q_k\|_{(n)} \|S_{n-k}\|_{(n+1)} .$$

Hence we get the following estimate for all $n = 0, \dots, J-1$:

$$\|Q_{n+1}\|_{(n+1)} \le \frac{C_\delta}{n+1} \sum_{k=0}^{n} \|Q_k\|_{(k)} \|S_{n-k}\|_{(n-k+1)} . \qquad (4.8)$$

Let us denote, for $n \in \mathbb{N}^*$,

$$G_n^1 = \sum_{\{p+q+r=n|q\neq n\}} \frac{(ihV)^p}{p!} e^{-ih\Delta} S_q e^{ih\Delta} \frac{(-ihV)^r}{r!}$$

$$\text{and} \qquad G_n^2 = - \sum_{\{p+q+r=n|q\neq n\}} Q_p^* X_q Q_r$$

the two members of the right hand side of the equation (3.10). Lemma 4.2 implies that we have, for $n = 1, \dots, J$,

$$\begin{aligned} \|G_n^1\|_{(n)} &\le \sum_{\{p+q+r=n|q\neq n\}} \frac{1}{p!\,r!} \|(ihV)^p e^{-ih\Delta} S_q e^{ih\Delta} (-ihV)^r\|_{(n)} \\ &\le C_\delta \sum_{\{p+q+r=n|q\neq n\}} \frac{1}{p!\,r!} \|(ihV)^p\|_{(n-1)} \|e^{-ih\Delta} S_q e^{ih\Delta} (-ihV)^r\|_{(n)} . \end{aligned}$$

Since the coefficients of the diagonal operators $e^{\pm ih\Delta}$ are of modulus one, Lemma 4.2 yields

$$\begin{aligned} \|G_n^1\|_{(n)} &\le C_\delta^2 \sum_{\{p+q+r=n|q\neq n\}} \frac{1}{p!\,r!} \|(ihV)^p\|_{(n-1)} \|S_q\|_{(n)} \|(-ihV)^r\|_{(n-1)} \\ &\le C_\delta^2 \sum_{\{p+q+r=n|q\neq n\}} \frac{1}{p!\,r!} \|(ihV)^p\|_{(0)} \|S_q\|_{(q+1)} \|(-ihV)^r\|_{(0)} . \end{aligned}$$

Using the hypothesis on V, we obtain for all $n = 1, \dots, J$,

$$\|G_n^1\|_{(n)} \le C_\delta^2 \sum_{\{p+q+r=n|q\neq n\}} \frac{(hM_V)^{p+r}}{p!r!} \|S_q\|_{(q+1)} . \qquad (4.9)$$

Similarly, for $n = 1, \dots, J$, we have

$$\begin{aligned} \|G_n^2\|_{(n)} &\le \sum_{\{p+q+r=n|q\neq n\}} \|Q_p^* X_q Q_r\|_{(n)} \\ &\le 2C_\delta \|Q_n\|_{(n)} \|X_0\|_{(n-1)} \\ &\quad + C_\delta^2 \sum_{\{p+q+r=n|p,q,r\neq n\}} \|Q_p\|_{(n-1)} \|X_q\|_{(n)} \|Q_r\|_{(n-1)} . \end{aligned}$$

Since $C_\delta > 1$, we can write

$$\|G_n^2\|_{(n)} \leq C_\delta^2 \sum_{\{p+q+r=n|q\neq n\}} \|Q_p\|_{(p)} \|X_q\|_{(q)} \|Q_r\|_{(r)}. \tag{4.10}$$

Now using Proposition (3.2) for the I_K-solution of (3.10) we have for $n = 1, \ldots, J$,

$$\|S_n\|_{(n+1)} \leq \frac{K^\nu}{\gamma h}\left(\frac{4\nu}{e\delta}\right)^{2\nu}\left(\|G_n^1\|_{(n)} + \|G_n^2\|_{(n)}\right) \tag{4.11}$$

$$\text{and} \qquad \|X_n\|_n \leq \|G_n^1\|_{(n)} + \|G_n^2\|_{(n)}. \tag{4.12}$$

These estimates, together with (4.8), (4.9) and (4.10) give recursive relations between the coefficients $(\|S_j\|_{j+1})_{0\leq j\leq J}$, $(\|Q_j\|_j)_{0\leq j\leq J}$ and $(\|X_j\|_j)_{0\leq j\leq J}$.
Let us define the numbers $(\mathsf{s}_j)_{j\geq 0}$, $(\mathsf{q}_j)_{j\geq 0}$ and $(\mathsf{x}_j)_{j\geq 0}$ as follows:

$$\mathsf{s}_0 = M_V \frac{K^\nu}{\gamma}\left(\frac{4\nu}{e\delta}\right)^{2\nu}, \quad \mathsf{q}_0 = 1 \quad \text{and} \quad \mathsf{x}_0 = hM_V,$$

and for all $n \in \mathbb{N}^*$, with $\kappa = \frac{K^\nu}{\gamma h}\left(\frac{4\nu}{e\delta}\right)^{2\nu}$,

$$\begin{aligned}
\mathsf{s}_n &= \kappa C_\delta^2 \sum_{\{p+q+r=n|q\neq n\}} \left(\frac{(hM_V)^{p+r}}{p!r!}\mathsf{s}_q + \mathsf{q}_p\mathsf{q}_r\mathsf{x}_q\right), \\
\mathsf{q}_n &= \frac{C_\delta}{n}\sum_{k=0}^{n-1} \mathsf{q}_k \mathsf{s}_{n-k-1}, \\
\mathsf{x}_n &= C_\delta^2 \sum_{\{p+q+r=n|q\neq n\}} \left(\frac{(hM_V)^{p+r}}{p!r!}\mathsf{s}_q + \mathsf{q}_p\mathsf{q}_r\mathsf{x}_q\right).
\end{aligned}$$

By induction, using the equations (4.8), (4.9), (4.10) and (4.11) we have that for $j = 0, \ldots, J$,

$$\|S_j\|_{j+1} \leq \mathsf{s}_j, \quad \|Q_j\|_j \leq \mathsf{q}_j \quad \text{and} \quad \|X_j\|_j \leq \mathsf{x}_j.$$

We then define the corresponding power series

$$\begin{aligned}
\mathsf{s}(t) &= \sum_{n\geq 0} \mathsf{s}_n t^n, \\
\mathsf{q}(t) &= \sum_{n\geq 0} \mathsf{q}_n t^n, \\
\text{and} \qquad \mathsf{x}(t) &= \sum_{n\geq 0} \mathsf{x}_n t^n.
\end{aligned}$$

By definition of the coefficients of these series, we have the following formal identities:

$$\begin{aligned}
\left(1 - \kappa C_\delta^2 (e^{2hM_V t} - 1)\right)\mathsf{s}(t) - \mathsf{s}_0 &= \kappa C_\delta^2 \mathsf{x}(t)(\mathsf{q}(t)^2 - 1), \\
\mathsf{q}'(t) &= C_\delta \mathsf{s}(t)\mathsf{q}(t), \\
\mathsf{x}(t) &= \kappa^{-1}\mathsf{s}(t),
\end{aligned}$$

where q' denotes the derivative of q with respect to t. We then derive that $\mathsf{q}(t)$

is solution of the following ordinary differential equation

$$\mathsf{q}'(t) = \frac{\mathsf{s}_0 C_\delta \mathsf{q}(t)}{1 - C_\delta^2\big(\kappa(e^{2hM_V t} - 1) + (\mathsf{q}(t)^2 - 1)\big)} \quad \text{and} \quad \mathsf{q}(0) = 1. \tag{4.13}$$

The study of this equation will give us bounds on the coefficients q_j. It is clear with the previous equalities that for sufficiently small t, the function $\mathsf{s}(t)$, $\mathsf{q}(t)$ and $\mathsf{x}(t)$ are analytic in t. Moreover, the following Lemma, whose proof is given in Appendix, gives a bound for the radius of convergence of the corresponding power series:

Lemma 4.3 *Let us define*

$$K_0^\nu = \max\Big(1, \frac{\rho_V^{2(\nu-1)}\gamma}{4}\Big(\frac{e}{4\nu}\Big)^{2\nu}\Big) \quad \textit{and} \quad r^{-1} = 20hM_V\kappa C_\delta^3.$$

For all $K \geq K_0$ and $h \in (0,1)$ satisfying (1.7), the functions x, q and s are analytic in $(-r, r)$, and satisfy for all $t \in (-r, r)$ the estimates:

$$0 < \mathsf{s}(t) \leq \frac{5\sqrt{5}}{4}\kappa h M_V, \quad 0,8 < \mathsf{q}(t) \leq \frac{\sqrt{5}}{2} \quad \textit{and} \quad 0 < \mathsf{x}(t) \leq \frac{5\sqrt{5}}{4}hM_V.$$

End of proof of Proposition 4.1: Let us consider the functions $\mathsf{s}(z)$, $\mathsf{q}(z)$ and $\mathsf{x}(z)$ for complex numbers z. As the coefficients of the corresponding power series are non-negative, we have for example for all sufficiently small z, $|\mathsf{s}(z)| \leq \mathsf{s}(|z|)$ and similar inequalities for $\mathsf{q}(z)$ and $\mathsf{x}(z)$. The previous Lemma combined with Cauchy estimates then shows that for $j = J$, we have

$$\mathsf{s}_J \leq \frac{5\sqrt{5}}{4}\kappa h M_V (20hM_V\kappa C_\delta^3)^J = \frac{5\sqrt{5}}{4}20^J C_\delta^{3J}(\kappa h M_V)^{J+1}.$$

By (4.7) and the definition of δ, we have $C_\delta \leq 2e^{\rho_V}\delta^{-1}$. The previous inequality then yields (recall that $\kappa = \frac{K^\nu}{\gamma h}\left(\frac{4\nu}{e\delta}\right)^{2\nu}$):

$$\mathsf{s}_J \leq \frac{5\sqrt{5}}{4}\left(\frac{K^\nu}{\gamma}\left(\frac{4\nu}{e\delta}\right)^{2\nu}\right)^{J+1} M_V^{J+1} 20^J 2^{3J} e^{3J\rho_V}\delta^{-3J}$$

and we easily see that there exists a positive constant C depending on V, ρ_V, γ and ν such that

$$\mathsf{s}_J \leq C^J K^{\nu(J+1)}\delta^{-2\nu(J+1)-3J}.$$

As $\delta^{-1} = (2J+1)/\rho_V$ we can modify C to obtain

$$\mathsf{s}_J \leq C^J K^{\nu(J+1)}(2J+1)^{(2\nu+3)J+2\nu}.$$

Now, since we have $\|S_J\|_{\rho_V/3} \leq \|S_J\|_{(J+1)} \leq \mathsf{s}_J$, we obtain the result with $\alpha = 2\nu$ and $\beta = 4\nu + 3$ after modification of the constant C to become C_0.
The proof of the other estimates for $\|X_J\|_{\rho_V/3}$ and $\|Q_J\|_{\rho_V}$ can be obtained similarly from Lemma 4.3. This finishes the proof of Proposition 4.1 ■

Remark 4.4 The coefficients α and β given in Proposition 4.1 are clearly not optimal. For simplicity, we did not try to optimize them, as well as the constants C_0 and K_0. ■

5 Error estimates

5.1 Construction of the operators

Assume that $K \geq 1$ and $N \geq 1$ are given. Let us define the following polynomials in $\lambda \in \mathbb{R}$:

$$S^{[N]}(\lambda) = \sum_{0 \leq n \leq N} \lambda^n S_n \qquad \text{and} \qquad X^{[N]}(\lambda) = \sum_{0 \leq n \leq N} \lambda^n X_n \tag{5.1}$$

where the coefficients S_n and X_n are defined by the recursive I_K-solutions of (3.8)-(3.10). Proposition 4.1 shows that $S^{[N]}(\lambda)$ and $X^{[N]}(\lambda)$ are operators in the space $\mathcal{S}_{\rho_V/3}$ for all $\lambda \in \mathbb{R}$. Lemma 4.2 then shows that the multiplication by $S^{[N]}(\lambda)$ or $X^{[N]}(\lambda)$ defines a continuous linear mapping from $\mathcal{A}_{\rho_V/4}$ to itself.

Let us denote by $Q^{[N]}(\lambda)$ and $\Sigma^{[N]}(\lambda)$ the maximal solutions in $\mathcal{A}_{\rho_V/4}$ of the following Cauchy problems

$$\left\{ \begin{array}{l} i\partial_\lambda Q^{[N]}(\lambda) = Q^{[N]}(\lambda) S^{[N]}(\lambda), \\ Q^{[N]}(0) = \mathrm{Id}, \end{array} \right. \qquad \text{and} \qquad \left\{ \begin{array}{l} i\partial_\lambda \Sigma^{[N]}(\lambda) = \Sigma^{[N]}(\lambda) X^{[N]}(\lambda), \\ \Sigma^{[N]}(0) = e^{ih\Delta}. \end{array} \right. \tag{5.2}$$

Since $\lambda \mapsto S^{[N]}(\lambda)$ (resp. $\lambda \mapsto X^{[N]}(\lambda)$) is continuous from $\mathbb{R}$ to $\mathcal{A}_{\rho_V/3}$, $Q^{[N]}(\lambda)$ and $\Sigma^{[N]}(\lambda)$ are defined for all $\lambda \in \mathbb{R}$ and belong to the space $\mathcal{A}_{\rho_V/4}$.

By construction, the spaces $\mathcal{X}_\rho^K$ are invariant by multiplication. Combining this and Lemma 4.2 we see that the multiplication by $X^{[N]}(\lambda)$ defines a continuous linear operator from $\mathcal{X}^K_{\rho_V/4}$ to itself.

As $e^{ih\Delta} \in \mathcal{X}^M_{\rho_V/4}$ and as $\mathcal{X}^K_{\rho_V/4}$ is closed for $\|\cdot\|_{\rho_V/4}$, we have

$$\forall \lambda \in \mathbb{R}, \qquad \Sigma^{[N]}(\lambda) \in \mathcal{X}^K_{\rho_V/4}.$$

Since $X^{[N]}(\lambda)$ and $S^{[N]}(\lambda)$ are polynomial functions of λ, $\Sigma^{[N]}(\lambda)$ and $Q^{[N]}(\lambda)$ are convergent power series in λ on a neighborhood of 0.

Moreover, as for all λ the operator $S^{[N]}(\lambda)$ is symmetric, the function

$$\lambda \mapsto Z(\lambda) := Q^{[N]}(\lambda)^* Q^{[N]}(\lambda)$$

is solution of the following Cauchy problem in some suitable $\mathcal{A}$ space:

$$\left\{ \begin{array}{l} i\partial_\lambda Z(\lambda) = [Z(\lambda), S^{[N]}(\lambda)], \\ Z(0) = \mathrm{Id}. \end{array} \right.$$

This implies that for all $\lambda \in \mathbb{R}$, $Z(\lambda) = \mathrm{Id}$ and hence that $Q^{[N]}(\lambda)$ is a unitary operator for all λ. A similar argument using the symmetry of $X^{[N]}(\lambda)$ shows that $\Sigma^{[N]}(\lambda)$ also is a unitary operator.

Let us denote, for λ sufficiently small,

$$Q^{[N]}(\lambda) = \sum_{n=0}^{+\infty} Q_n^{[N]} \lambda^n \qquad \text{and} \qquad \Sigma^{[N]}(\lambda) = \sum_{n=0}^{+\infty} \Sigma_n^{[N]} \lambda^n$$

where for all $n \in \mathbb{N}$, $Q_n^{[N]}$ and $\Sigma_n^{[N]}$ are in $\mathcal{A}_{\rho_V/4}$ (the series are absolutely convergent in this space for λ sufficiently small).

For all $\lambda \in \mathbb{R}$, we can define the following operator in a convenient $\mathcal{A}$ space

$$R^{[N]}(\lambda) = Q^{[N]}(\lambda)L(\lambda)Q^{[N]}(\lambda)^* - \Sigma^{[N]}(\lambda). \tag{5.3}$$

Using Lemma 4.2, $R^{[N]}(\lambda) \in \mathcal{A}_{\rho_V/5}$ and in this space, $R^{[N]}(\lambda)$ is the sum of the following absolutely convergent power series in a neighborhood of 0:

$$R^{[N]}(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \left[\sum_{p+q+r=n} \left(Q_p^{[N]} e^{ih\Delta} \frac{(-ih)^q}{q!} V^q (Q_r^{[N]})^* \right) - \Sigma_n^{[N]} \right]. \tag{5.4}$$

Since $Q_0 = Q_0^{[N]} = \mathrm{Id}$, the equality (3.8) and the fact that $Q^{[N]}$ is defined by (5.2) ensure that

$$\forall\, n \in \{1, \dots, N\}, \qquad Q_n = Q_n^{[N]}.$$

Moreover, the operators $(S_n)_{n\in\mathbb{N}}$ and $(X_n)_{n\in\mathbb{N}}$ satisfy (3.10) for all $n \in \mathbb{N}$ by definition. Hence we have in a suitable $\mathcal{A}$ space,

$$S^{[N]} - L^* S^{[N]} L = hV - (Q^{[N]})^* X^{[N]} Q^{[N]} + \mathcal{O}(\lambda^{N+1}).$$

We deduce that

$$S^{[N]} - L^* S^{[N]} L = hV - (Q^{[N]})^* (\Sigma^{[N]})^* (i\partial_\lambda \Sigma^{[N]}) Q^{[N]} + \mathcal{O}(\lambda^{N+1})$$

by definition (5.2) of $\Sigma^{[N]}$, and the fact that this operator is unitary. Then, since $(\Sigma^{[N]})^* = (Q^{[N]}) L^* (Q^{[N]})^* - (R^{[N]})^*$, we have

$$\begin{aligned} LS^{[N]} - S^{[N]} L = hLV &- (Q^{[N]})^* (i\partial_\lambda \Sigma^{[N]}) Q^{[N]} \\ &+ L(Q^{[N]})^* R^{[N]} (i\partial_\lambda \Sigma^{[N]}) Q^{[N]} + \mathcal{O}(\lambda^{N+1}). \end{aligned}$$

Since $S^{[N]} = (Q^{[N]})^* (i\partial_\lambda Q^{[N]}) = (S^{[N]})^*$, we derive that

$$\begin{aligned} L(i\partial_\lambda Q^{[N]})^* Q^{[N]} - (Q^{[N]})^* (i\partial_\lambda Q^{[N]}) L = hLV &- (Q^{[N]})^* (i\partial_\lambda \Sigma^{[N]}) Q^{[N]} \\ &+ L(Q^{[N]})^* R^{[N]} (i\partial_\lambda \Sigma^{[N]}) Q^{[N]} + \mathcal{O}(\lambda^{N+1}). \end{aligned}$$

After left-multiplying this equality by $Q^{[N]}$ and right-multiplying by $(Q^{[N]})^*$, we get

$$\begin{aligned} &Q^{[N]} L (i\partial_\lambda Q^{[N]})^* - (i\partial_\lambda Q^{[N]}) L (Q^{[N]})^* \\ &- hQ^{[N]} e^{ih\Delta} V e^{-ih\lambda V} (Q^{[N]})^* + i\partial_\lambda \Sigma^{[N]} = Q^{[N]} L (Q^{[N]})^* R^{[N]} (i\partial_\lambda \Sigma^{[N]}) + \mathcal{O}(\lambda^{N+1}). \end{aligned}$$

This equality expresses that

$$i\partial_\lambda R^{[N]} = -Q^{[N]} L (Q^{[N]})^* R^{[N]} (i\partial_\lambda \Sigma^{[N]}) + \mathcal{O}(\lambda^{N+1}).$$

Noticing that $R^{[N]}(0) = e^{ih\Delta} - e^{ih\Delta} = 0$, we derive by induction that

$$\forall\, 0 \leq n \leq N+1, \qquad \partial_\lambda^n R^{[N]}(0) = 0.$$

Therefore, (5.4) simplifies to

$$R^{[N]}(\lambda) = \sum_{n>N+1}^{+\infty} \lambda^n \left[\sum_{p+q+r=n} \left(Q_p^{[N]} e^{ih\Delta} \frac{(-ih)^q}{q!} V^q (Q_r^{[N]})^* \right) - \Sigma_n^{[N]} \right] \tag{5.5}$$

with absolute convergence in $\mathcal{A}_{\rho_V/5}$.

5.2 Estimate for the remainder term

We give now an estimate for the term $R^{[N]}(\lambda)$. We first give estimates for the coefficients of the formal series $\Sigma^{[N]}$ and $Q^{[N]}$:

Lemma 5.1 *Using the previous notations, there exists a constant $C_1 \geq 1$ depending only on V, ρ_V, γ and ν such that for all $N \geq 1$, all $n \in \mathbb{N}^*$, all $K \geq K_0$, and all $h \in (0,1)$ satisfying* (1.7)*,*

$$\|\Sigma_n^{[N]}\|_{\rho_V/4} \leq h(C_1 K^\alpha N^\beta)^n \quad \textit{and} \tag{5.6}$$

$$\|Q_n^{[N]}\|_{\rho_V/4} \leq (C_1 K^\alpha N^\beta)^n \tag{5.7}$$

where $\alpha = 2\nu$ and $\beta = 4\nu + 3$ are given in Proposition 4.1*.*

Proof. Since $\Sigma_0^{[N]} = e^{ih\Delta}$, we have $\|\Sigma_0^{[N]}\|_{\rho_V/4} = 1$. Moreover, since $\Sigma_1^{[N]} = \Sigma_0^{[N]} X_0$, we have with (4.2) that $\|\Sigma_1^{[N]}\|_{\rho_V/4} \leq hM_V$. Hence (5.6) holds for $n = 1$ with a constant C_1 depending only on V and ρ_V (notice that $K \geq K_0 \geq 1$). Assume now that (5.6) holds with some constant C_1 and for all $k \leq n \in \mathbb{N}^*$. By definition of $\Sigma^{[N]}$ and the use Lemma 4.2, we have

$$\|\Sigma_{n+1}^{[N]}\|_{\rho_V/4} \leq \frac{C_{\rho_V/12}}{n+1} \sum_{k=0}^{\min(n,N)} \|\Sigma_{n-k}^{[N]}\|_{\rho_V/4} \|X_k\|_{\rho_V/3}.$$

Using the induction hypothesis and the estimate (4.4), we thus have

$$\|\Sigma_{n+1}^{[N]}\|_{\rho_V/4} \leq \frac{C_{\rho_V/12}}{n+1} \sum_{k=0}^{\min(n,N)} h(C_1 K^\alpha N^\beta)^{n-k} h(C_0 K^\alpha k^\beta)^k.$$

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

$$\begin{aligned}
\|\Sigma_{n+1}^{[N]}\|_{\rho_V/4} &\leq h(C_1 K^\alpha N^\beta)^n \frac{hC_{\rho_V/12}}{n+1} \sum_{k=0}^{\min(n,N)} \left(\frac{k}{N}\right)^{\beta k} \\
&\leq h(C_1 K^\alpha N^\beta)^n (hC_{\rho_V/12}) \frac{1}{n+1} \sum_{k=0}^{\min(n,N)} 1 \\
&\leq h(C_1 K^\alpha N^\beta)^{n+1}
\end{aligned}$$

provided that $C_1 \geq C_{\rho_V/12}$ and since $K \geq 1$. This shows (5.6).
The proof of (5.7) is similar using the estimate (4.3) instead of (4.4). ■

The previous Lemma yields the following estimates:

Proposition 5.2 *Using the previous notations, for all $K \geq K_0$, all $N \geq 1$, all $h \in (0,1)$ satisfying* (1.7) *and all $\lambda \in \mathbb{R}$ such that $|\lambda| \leq (2C_1K^\alpha N^\beta)^{-1}$, we have*

$$\|Q^{[N]}(\lambda) - \mathrm{Id}\|_{\rho_V/4} \leq 2C_1K^\alpha N^\beta|\lambda| \tag{5.8}$$

and

$$\|\Sigma^{[N]}(\lambda) - e^{ih\Delta}\|_{\rho_V/4} \leq 2hC_1K^\alpha N^\beta|\lambda|. \tag{5.9}$$

Proof. We have

$$Q^{[N]}(\lambda) - \mathrm{Id} = \sum_{n\geq 1} \lambda^n Q_n^{[N]}.$$

This implies, using (5.7)

$$\|Q^{[N]}(\lambda) - \mathrm{Id}\|_{\rho_V/4} \leq \sum_{n\geq 1}(|\lambda|C_1K^\alpha N^\beta)^n$$

and the result follows straightforwardly. The second inequality is proved similarly. ■

We now give an estimate for the remainder term itself. We use the following notation: For a function f defined in a neighborhood of 0 in $\mathbb{R}$ and such that for all $n \in \mathbb{N}$, the derivative $f^{(n)}(0)$ is defined, we set

$$T_N(f)(x) = f(x) - \sum_{p=0}^{\lfloor N\rfloor} x^p \frac{f^{(p)}(0)}{p!} \tag{5.10}$$

where $\lfloor\cdot\rfloor$ denotes the nearest integer towards minus infinity.

Proposition 5.3 *Using the notations of Proposition* 4.1*, there exists a constant $C_2 > 0$ depending only on V, ρ_V, γ and ν such that for all $h \in (0,1)$ satisfying* (1.7)*, all $N \geq 1$, all $K \geq K_0$ and all $\lambda \in \mathbb{R}$ such that $|\lambda| \leq (2C_1K^\alpha N^\beta)^{-1}$ we have*

$$\|R^{[N]}(\lambda)\|_{\rho_V/5} \leq (C_2|\lambda|K^{3\alpha}N^{3(\beta+1)})^N. \tag{5.11}$$

Proof. Using Lemma 4.2, the formula (5.5) yields for $\lambda \in \mathbb{R}$ sufficiently small,

$$\begin{aligned}
&\|R^{[N]}(\lambda)\|_{\rho_V/5} \\
&\leq \sum_{n\geq N+1}^{+\infty} |\lambda|^n \left[C_{\frac{\rho_V}{20}} \sum_{p+q+r=n} \Big(\|Q_p^{[N]}\|_{\rho_V/5} \, \| \frac{(-ih)^q}{q!} V^q (Q_r^{[N]})^* \|_{\rho_V/4} \Big) \right] \\
&\qquad + \sum_{n\geq N+1}^{+\infty} |\lambda|^n \|\Sigma_n^{[N]}\|_{\rho_V/5} \\
&\leq \sum_{n\geq N+1}^{+\infty} |\lambda|^n \left[C_{\frac{\rho_V}{20}} C_{\frac{\rho_V}{12}} \sum_{p+q+r=n} \Big(\|Q_p^{[N]}\|_{\rho_V/5} \, \frac{h^q}{q!} \|V^q\|_{\rho_V/3} \, \|(Q_r^{[N]})^*\|_{\rho_V/4} \Big) \right] \\
&\qquad + \sum_{n\geq N+1}^{+\infty} |\lambda|^n \|\Sigma_n^{[N]}\|_{\rho_V/5} \,.
\end{aligned}$$

Using Lemma 5.1 we thus get

$$\begin{aligned}
&\|R^{[N]}(\lambda)\|_{\rho_V/5} \\
&\leq \sum_{n\geq N+1}^{+\infty} |\lambda|^n \left[C_{\frac{\rho_V}{20}} C_{\frac{\rho_V}{12}} \sum_{p+q+r=n} \Big((C_1 K^\alpha N^\beta)^p \frac{h^q}{q!} M_V^q (C_1 K^\alpha N^\beta)^r \Big) \right] \\
&\qquad + h \sum_{n\geq N+1}^{+\infty} (|\lambda| C_1 K^\alpha N^\beta)^n.
\end{aligned}$$

For $x \in \mathbb{R}$ such that $|x| < (C_1 K^\alpha N^\beta)^{-1}$, we set

$$f(x) = (1 - C_1 K^\alpha N^\beta x)^{-1} \qquad \text{and} \qquad g(x) = e^{h M_V x}.$$

The previous inequality can then be written

$$\|R_N(\lambda)\|_{\rho_V/5} \leq C_{\frac{\rho_V}{20}} C_{\frac{\rho_V}{12}} T_N(f^2 g)(|\lambda|) + h T_N(f)(|\lambda|)$$

where T_N is defined in (5.10). Now for all $p \in \mathbb{N}$ and all $x \in \mathbb{R}$ such that $|x| < (C_1 K^\alpha N^\beta)^{-1}$, we have

$$\frac{\mathrm{d}^p f}{\mathrm{d}x^p}(x) = \frac{p\,!\,(C_1 K^\alpha N^\beta)^p}{(1 - C_1 K^\alpha N^\beta x)^{p+1}}$$

and

$$\frac{\mathrm{d}^p (f^2)}{\mathrm{d}x^p}(x) = \frac{(p+1)!\,(C_1 K^\alpha N^\beta)^p}{(1 - C_1 K^\alpha N^\beta x)^{p+2}},$$

and for the function g:

$$\frac{\mathrm{d}^p g}{\mathrm{d}x^p}(x) = (h M_V)^p e^{h M_V x}.$$

By definition of T_N, and as f and g are smooth, we have for $|\lambda| \leq (2C_1K^\alpha N^\beta)^{-1}$,

$$\begin{aligned} T_N(f^2g)(|\lambda|) &\leq \frac{|\lambda|^{\lfloor N\rfloor+1}}{(\lfloor N\rfloor+1)!} \sup_{|t|\leq(2C_1K^\alpha N^\beta)^{-1}} \left|\frac{\mathrm{d}^{\lfloor N\rfloor+1}(f^2g)}{\mathrm{d}x^{\lfloor N\rfloor+1}}(t)\right| \\ \text{and} \quad T_N(f)(|\lambda|) &\leq \frac{|\lambda|^{\lfloor N\rfloor+1}}{(\lfloor N\rfloor+1)!} \sup_{|t|\leq(2C_1K^\alpha N^\beta)^{-1}} \left|\frac{\mathrm{d}^{\lfloor N\rfloor+1}f}{\mathrm{d}x^{\lfloor N\rfloor+1}}(t)\right|. \end{aligned}$$

As for $|t| \leq (2C_1K^\alpha N^\beta)^{-1}$ we have

$$\left|\frac{\mathrm{d}^{\lfloor N\rfloor+1}f}{\mathrm{d}x^{\lfloor N\rfloor+1}}(t)\right| = \frac{(\lfloor N\rfloor+1)!\,(C_1K^\alpha N^\beta)^{\lfloor N\rfloor+1}}{(1-C_1K^\alpha N^\beta t)^{\lfloor N\rfloor+2}} \leq 2(\lfloor N\rfloor+1)!(2C_1K^\alpha N^\beta)^{\lfloor N\rfloor+1},$$

we derive that (notice that $|\lambda| \leq 1/2 \leq 1$)

$$\begin{aligned} T_N(f)(|\lambda|) &\leq 2(2C_1K^\alpha N^\beta|\lambda|)^{\lfloor N\rfloor+1} \\ &\leq (4C_1K^\alpha N^\beta)^{N+1}|\lambda|^N \\ &\leq (16C_1^2K^{2\alpha}N^{2\beta})^N|\lambda|^N. \end{aligned}$$

Similarly, for $|t| \leq (2C_1K^\alpha N^\beta)^{-1}$ we have

$$\frac{\mathrm{d}^{\lfloor N\rfloor+1}(f^2g)}{\mathrm{d}x^{\lfloor N\rfloor+1}}(t) = \sum_{k=0}^{\lfloor N\rfloor+1} \frac{(\lfloor N\rfloor+1)!}{k!(\lfloor N\rfloor+1-k)!}\left(\frac{\mathrm{d}^kf^2}{\mathrm{d}x^k}(t)\right)\left(\frac{\mathrm{d}^{\lfloor N\rfloor+1-k}g}{\mathrm{d}x^{\lfloor N\rfloor+1-k}}(t)\right)$$

and hence

$$\begin{aligned} &\left|\frac{\mathrm{d}^{\lfloor N\rfloor+1}(f^2g)}{\mathrm{d}x^{\lfloor N\rfloor+1}}(t)\right| \\ &\leq \sum_{k=0}^{\lfloor N\rfloor+1} \frac{(\lfloor N\rfloor+1)!}{k!(\lfloor N\rfloor+1-k)!}\left(\frac{(k+1)!\,(C_1K^\alpha N^\beta)^k}{(1-C_1K^\alpha N^\beta t)^{k+2}}\right)(hM_V)^{\lfloor N\rfloor+1-k}e^{hM_Vt}. \end{aligned}$$

As $|t| \leq (2C_1K^\alpha N^\beta)^{-1}$ and as we can always assume that $hM_V \leq M_V \leq C_1$ with $C_1 \geq 1$, the right hand side of the previous equation is bounded by

$$4e^{hM_Vt}C_1^{\lfloor N\rfloor+1}(\lfloor N\rfloor+1)!\sum_{k=0}^{\lfloor N\rfloor+1}\frac{k+1}{(\lfloor N\rfloor+1-k)!}\left(2C_1K^\alpha N^\beta\right)^k$$

and hence by

$$4\sqrt{e}(C_1)^{\lfloor N\rfloor+1}(\lfloor N\rfloor+1)!(\lfloor N\rfloor+1)\sum_{k=0}^{\lfloor N\rfloor+1}\left(2C_1K^\alpha N^\beta\right)^k,$$

using the fact that $|hM_Vt| \leq 1/2$. The last factor is equal to

$$\frac{(2C_1K^\alpha N^\beta)^{\lfloor N\rfloor+2}-1}{2C_1K^\alpha N^\beta-1}.$$

Since $C_1K^\alpha N^\beta \geq 1$, this ratio is bounded by

$$(2C_1K^\alpha N^\beta)^{\lfloor N\rfloor+2}.$$

This yields

$$\left|\frac{\mathrm{d}^{\lfloor N\rfloor+1}(f^2g)}{\mathrm{d}x^{\lfloor N\rfloor+1}}(t)\right| \leq 4\sqrt{e}(C_1)^{\lfloor N\rfloor+1}(\lfloor N\rfloor+1)!(\lfloor N\rfloor+1)(2C_1K^\alpha N^\beta)^{\lfloor N\rfloor+2}$$

and hence for $|\lambda| \leq (2C_1K^\alpha N^\beta)^{-1}$,

$$\begin{aligned} T_N(f^2g)(|\lambda|) &\leq 4\sqrt{e}|\lambda|^{\lfloor N\rfloor+1}\left(2C_1^2K^\alpha(\lfloor N\rfloor+1)^{\beta+1}\right)^{\lfloor N\rfloor+2} \\ &\leq |\lambda|^N(8eC_1^2K^\alpha(2N)^{\beta+1})^{N+2} \\ &\leq |\lambda|^N(2^{3(\beta+4)}e^3C_1^6K^{3\alpha}N^{3(\beta+1)})^N. \end{aligned}$$

Collecting the previous estimates, we get (5.11) for a suitable constant C_2. ■

We are now able to prove Theorem 2.2:

Proof of Theorem 2.2. Let $h \in (0,1)$ be a stepsize satisfying (1.7) and consider positive numbers σ_N and σ_K such that

$$\alpha\sigma_K + (\beta+1)\sigma_N \leq 1/4. \tag{5.12}$$

For example, $\sigma_N = \sigma_K = 1/(8\max(\alpha,\beta+1)) = 1/(32(\nu+1)) > 0$ is a possible choice of parameters. We make this specific choice to prove Theorem 2.2. For these parameters, we set for all $\lambda \in (0,1)$,

$$K = \lambda^{-\sigma_K} \quad \text{and} \quad N = 1/(2C_1)^{1/\beta}\lambda^{-\sigma_N} \tag{5.13}$$

and we define

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

Since $\sigma_N = \sigma_K > 0$ and C_1 only depends on V, γ and ν, there exists $\lambda_0 \in (0,1)$ depending only on V, ρ_V, γ and ν such that for all $\lambda \in (0,\lambda_0)$, we have $K = \lambda^{-\sigma_N} \geq K_0$ and $N = 1/(2C_1)^{1/\beta}\lambda^{-\sigma_N} \geq 1$. For such a λ, we have

$$(2C_1K^\alpha N^\beta)^{-1} = \lambda^{\alpha\sigma_K+\beta\sigma_N} \geq \lambda$$

since $\alpha\sigma_K + \beta\sigma_N \leq 1$ with (5.12) and $\lambda \leq 1$.

Therefore, Proposition 5.2 ensures that

$$\|Q(\lambda) - \mathrm{Id}\|_{\rho_V/4} \leq \lambda^{1-(\alpha\sigma_K+\beta\sigma_N)} \leq \lambda^{1/2}$$

and

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

Moreover, Proposition 5.3 ensures that

$$\|R(\lambda)\|_{\rho_V/5} \leq (C_2C_1^{-3(\beta+1)/\beta}\lambda^{1-(3\alpha\sigma_K+3(\beta+1)\sigma_N})^N.$$

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

$$1 - (3\alpha\sigma_K + 3(\beta+1)\sigma_N \geq 1/4 > 0$$

by (5.12), after a possible decrease of λ_0 (depending only on V, ρ_V, γ and ν again[4]), we can assume that

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

Therefore, we get eventually that for all $\lambda \in (0, \lambda_0)$,

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

and this finishes the proof of the Theorem. ■

6 Proof of the corollary

Before starting the proof of Corollary 2.3, we give the following two lemmas:

Lemma 6.1 *Let $\mu > 0$. Assume that $R \in \mathcal{A}_\mu$. Let $\varphi \in L^2(\mathbb{T})$ and let $\psi = R\varphi$. Then for all $k \in \mathbb{Z}$, we have*

$$|\psi_k| \leq |\psi|_{|k|} \leq \|\psi\| \leq C_\mu \|R\|_\mu \|\varphi\|$$

where $\|\cdot\|$ is the L^2-norm for functions and where $\|\cdot\|_\mu$ is the norm (2.2) *for operators. Recall that the value of the constant C_μ is given in Lemma* 4.2.

Proof. By definition, we have for all $k \in \mathbb{Z}$,

$$\psi_k = \sum_{\ell \in \mathbb{Z}} R_{k\ell} \varphi_\ell.$$

Hence, we have with the Cauchy-Schwarz inequality

$$\begin{aligned}
\|\psi\|^2 &\leq \sum_{k\in\mathbb{Z}} \Big| \sum_{\ell\in\mathbb{Z}} |R_{k\ell}||\varphi_\ell| \Big|^2 \\
&\leq \|R\|_\mu^2 \sum_{k\in\mathbb{Z}} \Big| \sum_{\ell\in\mathbb{Z}} e^{-\frac{\mu}{2}|k-\ell|} |\varphi_\ell| \, e^{-\frac{\mu}{2}|k-\ell|} \Big|^2 \\
&\leq \|R\|_\mu^2 \sum_{k\in\mathbb{Z}} \left[\Big(\sum_{p\in\mathbb{Z}} e^{-\mu|k-p|} \Big) \Big(\sum_{\ell\in\mathbb{Z}} e^{-\mu|k-\ell|} |\varphi_\ell|^2 \Big) \right].
\end{aligned}$$

Using (4.7), we see that

$$\begin{aligned}
\|\psi\|^2 &\leq \|R\|_\mu^2 C_\mu \sum_{\ell\in\mathbb{Z}} |\varphi_\ell|^2 \sum_{k\in\mathbb{Z}} e^{-\mu|k-\ell|} \\
&\leq \|R\|_\mu^2 C_\mu^2 \|\varphi\|^2
\end{aligned}$$

and this yields the result using the fact that for all $k \in \mathbb{Z}$,

$$|\psi_k| \leq |\psi|_{|k|} \leq \|\psi\|.$$

■

[4]We recall that C_2 only depends on V, γ and ν by Proposition 5.3

Lemma 6.2 *Let $\rho > 0$ and $s \geq 0$ be real numbers. There exists a positive constant C depending only on ρ and s such that for all $A \in \mathcal{A}_\rho$ and all φ such that $\|\varphi\|_{s,\infty} < \infty$, we have*

$$\|A\varphi\|_{s,\infty} \leq C\|A\|_\rho \|\varphi\|_{s,\infty}$$

Proof. By definition of $\|\cdot\|_{s,\infty}$ (see (2.11)), we have

$$\forall\, k \in \mathbb{N}, \quad |\varphi|_k \leq \|\varphi\|_{s,\infty} (1+k)^{-s}.$$

We deduce that for all $k \in \mathbb{Z}$

$$\begin{aligned} |(A\varphi)_k| &\leq \sum_{\ell\in\mathbb{Z}} \|A\|_\rho e^{-\rho|k-\ell|}|\varphi_\ell| \\ &\leq \|A\|_\rho \|\varphi\|_{s,\infty} \sum_{\ell\in\mathbb{Z}} e^{-\rho|k-\ell|}(1+|\ell|)^{-s}. \end{aligned}$$

so that

$$\begin{aligned} (1+|k|)^s|(A\varphi)_k| &\leq \|A\|_\rho \|\varphi\|_{s,\infty} \sum_{\ell\in\mathbb{Z}} e^{-\rho|k-\ell|} \left(\frac{1+|k|}{1+|\ell|}\right)^s \\ &\leq \|A\|_\rho \|\varphi\|_{s,\infty} \sum_{\ell\in\mathbb{Z}} e^{-\rho|k-\ell|} \left(\frac{1+|k-\ell|+|\ell|}{1+|\ell|}\right)^s \\ &\leq \|A\|_\rho \|\varphi\|_{s,\infty} \sum_{\ell\in\mathbb{Z}} e^{-\rho|k-\ell|} (1+|k-\ell|)^s \end{aligned}$$

and it is clear that the last sum is finite and independent on k. ■

We now begin the proof of the Corollary 2.3. We first show (i), then (iii) and finally (ii).

Proof of (i). It is clear that we have for all $n \geq 1$,

$$\|\varphi^n\| = \|\varphi^0\|.$$

With the notations of Theorem 2.2, let $\psi^n = Q(\lambda)\varphi^n$. As $Q(\lambda)$ is unitary we hence also have

$$\|\psi^n\| = \|\psi^0\| = \|\varphi^0\|.$$

Moreover, by (2.6), we have for all $n \geq 0$,

$$\psi^{n+1} = (\Sigma(\lambda) + R(\lambda))\psi^n$$

Now the fact that $\Sigma(\lambda)$ is an almost X-shaped unitary operator implies that for $0 \leq k \leq K = \lambda^{-\sigma}$, we have

$$|\Sigma(\lambda)\psi^n|_k = |\psi^n|_k.$$

We thus have for all $0 \leq k \leq K$,

$$\begin{aligned} \big|\,|\psi^{n+1}|_k - |\psi^n|_k\big| &= \big|\,|\psi^{n+1}|_k - |\Sigma(\lambda)\psi^n|_k\big| \\ &\leq |\psi^{n+1} - \Sigma(\lambda)\psi^n|_k \\ &\leq |R(\lambda)\psi^n|_k. \end{aligned}$$

Recall that $|R(\lambda)\psi^n|_k^2 = |(R(\lambda)\psi^n)_k|^2 + |(R(\lambda)\psi^n)_{-k}|^2$. Using lemma 6.1 with $\mu = \rho_V/5$, we thus have

$$\begin{aligned} \big|\, |\psi^{n+1}|_k - |\psi^n|_k \big| &\leq \sqrt{2} C_{\rho_V/5} \|R(\lambda)\|_{\rho_V/5} \|\psi^n\| \\ &\leq \sqrt{2} C_{\rho_V/5} \exp(-c\lambda^{-\sigma}) \|\varphi^0\| \, . \end{aligned}$$

Hence for $n \leq \exp(c\lambda^{-\sigma}/2)$ we have by triangle inequality,

$$\big|\, |\psi^n|_k - |\psi^0|_k \big| \leq \sqrt{2} C_{\rho_V/5} \exp(-c\lambda^{-\sigma}/2) \|\varphi^0\| \, . \tag{6.1}$$

For all $0 \leq k \leq \lambda^{-\sigma}$, this inequality shows the extremely good conservation of the oscillatory energy $|\psi^n|_k$.
Now using the estimate (2.5) and Lemma 6.1, we get for all $(n,k) \in \mathbb{N}^2$,

$$\begin{aligned} |\varphi^n - \psi^n|_k &= |(\mathrm{Id} - Q(\lambda))\varphi^n|_k \\ &\leq \lambda^{1/2} \|\varphi^n\| \\ &\leq \lambda^{1/2} \|\varphi^0\| \, . \end{aligned}$$

Therefore, for all n and k,

$$\begin{aligned} \Big| \big||\varphi^n|_k - |\varphi^0|_k\big| - \big||\psi^n|_k - |\psi^0|_k\big| \Big| &\leq \Big| \big(|\varphi^n|_k - |\varphi^0|_k\big) - \big(|\psi^n|_k - |\psi^0|_k\big) \Big| \\ &\leq |\varphi^n - \psi^n|_k + |\varphi^0 - \psi^0|_k \\ &\leq 2\lambda^{1/2} \|\varphi^0\| \, . \end{aligned}$$

We thus deduce that for all $n \leq \exp(c\lambda^{-\sigma}/2)$ and all $k \leq \lambda^{-\sigma}$,

$$\begin{aligned} \big||\varphi^n|_k - |\varphi^0|_k\big| &\leq \big||\psi^n|_k - |\psi^0|_k\big| + 2\lambda^{1/2} \|\varphi^0\| \\ &\leq 2\lambda^{1/2} \|\varphi^0\| + \sqrt{2} C_{\rho_V/5} \exp(-c\lambda^{-\sigma}/2) \|\varphi^0\| \, , \end{aligned}$$

so that (2.12) is proved. ■

Proof of (iii). Recall that λ is chosen in $(0, \lambda_0)$ and that $K = \lambda^{-\sigma}$ with the notations of Theorem 2.2. For a function φ, we set

$$(\pi_K \varphi)(x) = \sum_{|k|>K} \varphi_k e^{inkx}. \tag{6.2}$$

The structure of $\Sigma(\lambda)$ implies that $[\pi_K, \Sigma(\lambda)] = 0$. Hence, we have

$$\|\pi_K \Sigma(\lambda)\varphi\| = \|\pi_K \varphi\| \, .$$

Moreover, Theorem 2.2 ensures that $\|R(\lambda)\|_{\rho_V/5} \leq \exp(-c\lambda^{-\sigma})$, so using lemma 6.1 we have

$$\|\pi_K R(\lambda)\varphi\| \leq \|R(\lambda)\varphi\| \leq C_{\rho_V/5} \exp(-c\lambda^{-\sigma}) \|\varphi\| \, .$$

Therefore, for all $n \in \mathbb{N}$, we have

$$\begin{aligned} \big| \|\pi_K \psi^{n+1}\| - \|\pi_K \psi^n\| \,\big| &= \big| \|\pi_K \psi^{n+1}\| - \|\pi_K \Sigma(\lambda)\psi^n\| \,\big| \\ &\leq \|\pi_K \big(\psi^{n+1} - \Sigma(\lambda)\psi^n\big)\| \\ &\leq \|\pi_K R(\lambda)\psi^n\| \\ &\leq C_{\rho_V/5} \exp(-c\lambda^{-\sigma})\|\psi^n\| \\ &\leq C_{\rho_V/5} \exp(-c\lambda^{-\sigma})\|\varphi^0\| \,. \end{aligned}$$

Hence, we have by triangle inequality for $n \leq \exp(c\lambda^{-\sigma}/2)$,

$$\big| \|\pi_K \psi^n\| - \|\pi_K \psi^0\| \,\big| \leq C_{\rho_V/5} \exp(-c\lambda^{-\sigma}/2)\|\varphi^0\| \,. \tag{6.3}$$

Let $\rho \in (0, \rho_V/5)$ and assume that $\varphi^0 \in U_\rho$. Notice that we have

$$\|\varphi^0\|^2 = \sum_{k\in\mathbb{Z}} |\varphi^0_k|^2 \leq \|\varphi^0\|_\rho^2 C_{2\rho}. \tag{6.4}$$

Since $\psi^0 = Q(\lambda)\varphi^0$, Lemma 4.2 ensures that

$$\|\psi^0\|_\rho \leq C_{\rho_V/5-\rho} \|Q(\lambda)\|_{\rho_V/5} \|\varphi^0\|_\rho \,.$$

Moreover, since $\|Q(\lambda)\|_{\rho_V/5} \leq (1 + \lambda_0^{1/2})$ by Theorem 2.2, we derive that there exists a constant $C > 0$ depending only on V, ρ_V, γ, ν, and ρ such that

$$\forall k \in \mathbb{Z}, \qquad |\psi^0_k| \leq C\|\varphi^0\|_\rho e^{-\rho|k|}.$$

Therefore,

$$\begin{aligned} \|\pi_K \psi^0\|^2 &\leq C^2 \|\varphi^0\|_\rho^2 \sum_{|k|>K} e^{-2\rho_k} \\ &\leq C^2 \|\varphi^0\|_\rho^2 e^{-2\rho\lambda^{-\sigma}} 2 \sum_{k=0}^{\infty} e^{-2\rho|k|}. \end{aligned}$$

Hence, after a possible increase of C, we get

$$\|\pi_K \psi^0\| \leq C\|\varphi^0\|_\rho \exp(-\rho\lambda^{-\sigma}).$$

Then, using (6.3) and (6.4), we get, after another possible increase of C, for all $n \leq \exp(c\lambda^{-\sigma}/2)$,

$$\|\pi_K \psi^n\| \leq C \exp(-c'\lambda^{-\sigma})\|\varphi^0\|_\rho \tag{6.5}$$

where $c' = \min(c/2, \rho) > 0$ only depends on V, γ, ν, and ρ.
Moreover, the inequality (6.1) shows that for $0 \leq k \leq \lambda^{-\sigma}$ and all $n \leq \exp(c\lambda^{-\sigma}/2)$, we have for all $\mu > 0$,

$$e^{\mu k} \big| |\psi^n|_k - |\psi^0|_k \big| \leq \sqrt{2} C_{\rho_V/5} \exp(\mu K - c\lambda^{-\sigma}/2)\|\varphi^0\| \,,$$

so that if we set $\mu_0 = c'/2 > 0$, we have for $\mu \in (0, \mu_0)$,

$$\sup_{0\leq k\leq\lambda^{-\sigma}} \Big(e^{\mu k} \big| |\psi^n|_k - |\psi^0|_k \big| \Big) \leq C' \exp(-c'\lambda^{-\sigma}/2)\|\varphi^0\| \tag{6.6}$$

with $C' = \sqrt{2}C_{\rho_V/5}$, since $\mu - c/2 \leq -\mu_0 = -c'/2$.

Recall that for all $n \in \mathbb{N}$, $\varphi^n = Q(\lambda)^* \psi^n$. Using the decomposition

$$\psi^n = (\mathrm{Id} - \pi_K)\psi^n + \pi_K \psi^n$$

we thus have

$$\varphi^n = Q(\lambda)^*(\mathrm{Id} - \pi_K)\psi^n + Q(\lambda)^* \pi_K \psi^n$$

and therefore

$$\varphi^n - \psi^n = (Q(\lambda)^* - \mathrm{Id})(\mathrm{Id} - \pi_K)\psi^n + (Q(\lambda)^* - \mathrm{Id})\pi_K \psi^n. \tag{6.7}$$

Using Lemma 6.1 and estimate (2.5), we get for $0 \leq k \leq \lambda^{-\sigma}$,

$$\begin{aligned} \big| |\varphi^n|_k - |\psi^n|_k \big| &\leq |\varphi^n - \psi^n|_k \\ &\leq |(Q(\lambda)^* - \mathrm{Id})(\mathrm{Id} - \pi_K)\psi^n|_k + |(Q(\lambda)^* - \mathrm{Id})\pi_K \psi^n|_k \\ &\leq |(Q(\lambda)^* - \mathrm{Id})(\mathrm{Id} - \pi_K)\psi^n|_k + C_{\rho_V/4}\lambda^{1/2}\|\pi_K \psi^n\| \,. \end{aligned}$$

On one hand, we have with (6.5) that for all $\mu \in (0, \mu_0)$, all $n \leq \exp(c\lambda^{-\sigma}/2)$ and all $k \leq \lambda^{-\sigma}$,

$$\|\pi_K \psi^n\| \, e^{+\mu k} \leq C \exp(-c'\lambda^{-\sigma}/2) \|\varphi^0\|_\rho \tag{6.8}$$

since $\mu - c' \leq -c'/2$.
On the other hand, with Lemma 4.2 and Theorem 2.2, we have

$$\|(Q(\lambda)^* - \mathrm{Id})(\mathrm{Id} - \pi_K)\psi^n\|_\mu \leq C_{\rho_V/4-\mu}\lambda^{1/2}\|(\mathrm{Id} - \pi_K)\psi^n\|_\mu$$

and the inequalities (6.6) and (6.4) ensure that for all $n \leq \exp(c\lambda^{-\sigma}/2)$,

$$\begin{aligned} \|(\mathrm{Id} - \pi_K)\psi^n\|_\mu &\leq \sqrt{2}\|\psi^0\|_\mu + C' \exp(-c'\lambda^{-\sigma}/2)\|\varphi^0\| \\ &\leq C\|\varphi^0\|_\rho \end{aligned}$$

after a possible increase of C (still depending only on V, ρ_V, γ, ν and ρ).
As a conclusion, after another possible increase of C, we get for all $n \leq \exp(c\lambda^{-\sigma}/2)$, all $k \leq \lambda^{-\sigma}$ and all $\mu \in (0, \mu_0)$,

$$\big| |\varphi^n|_k - |\psi^n|_k \big| e^{+\mu k} \leq C\lambda^{1/2}\|\varphi^0\|_\rho \,. \tag{6.9}$$

Eventually, we get for all $n \leq \exp(c\lambda^{-\sigma}/2)$, all $k \leq \lambda^{-\sigma}$ and all $\mu \in (0, \mu_0)$

$$\begin{aligned} &e^{\mu k}\big| |\varphi^n|_k - |\varphi^0|_k \big| \\ &\leq e^{\mu k}\big| |\varphi^n|_k - |\psi^n|_k \big| + e^{\mu k}\big| |\psi^n|_k - |\psi^0|_k \big| + e^{\mu k}\big| |\psi^0|_k - |\varphi^0|_k \big| \\ &\leq C\lambda^{1/2}\|\varphi^0\|_\rho \end{aligned}$$

after a last increase of C, using (6.9), (6.6) and the fact that

$$\|\psi^0 - \varphi^0\|_\mu \leq \|\psi^0 - \varphi^0\|_\rho \leq C_{\rho_V/4-\rho}\|\varphi^0\|_\rho$$

by Lemma 4.2. This proves (2.14) and hence (iii). ∎

Proof of (ii). With the notations of Theorem 2.2 and Corollary 2.3, we assume that $h \in (0, 1)$ satisfying (1.7), $\lambda \in (0, \lambda_0)$ and $s > 1/2$ are given real numbers.

Theorem 2.2 and Lemma 6.2 ensure that there exists a positive constant c_s depending only on V, ρ_V, γ, ν and s such that

$$\forall k \in \mathbb{N}, \qquad |\psi^0|_k \le c_s \|\varphi^0\|_{s,\infty} (1+k)^{-s}.$$

Note that, since $s > 1/2$, we have

$$\|\varphi^0\| = \Big(\sum_{k\in\mathbb{N}} |\varphi^0|_k^2\Big)^{1/2} \le \Big(\sum_{p\in\mathbb{N}} (1+p)^{-2s}\Big)^{1/2} \|\varphi^0\|_{s,\infty} < +\infty$$

and similarly

$$\begin{aligned} \|\pi_K \psi^0\|^2 &= \sum_{k>K} |\psi^0|_k^2 \\ &\le c_s^2 \|\varphi^0\|_{s,\infty}^2 \sum_{k>K} (1+k)^{-2s} \\ &\le c_s^2 \|\varphi^0\|_{s,\infty}^2 \int_{K-1}^{+\infty} (1+t)^{-2s}\,\mathrm{d}t \\ &\le c_s^2 \|\varphi^0\|_{s,\infty}^2 \frac{K^{-(2s-1)}}{2s-1} \\ &\le c_s^2 \|\varphi^0\|_{s,\infty}^2 \frac{\lambda^{\sigma(2s-1)}}{2s-1} \end{aligned}$$

which reads

$$\|\pi_K \psi^0\| \le c_s \|\varphi^0\|_{s,\infty} \lambda^{\sigma(s-1/2)}$$

after a possible increase of the constant c_s.
Another possible increase of the constant c_s allows us to write, using (6.3), that for $n \le \exp(c\lambda^{-\sigma}/2)$,

$$\begin{aligned} \|\pi_K \psi^n\| &\le C_{\rho_V/5} \exp(-c\lambda^{-\sigma}/2) \|\varphi^0\| + \|\pi_K \psi^0\| \\ &\le c_s \exp(-c\lambda^{-\sigma}/2) \|\varphi^0\|_{s,\infty} + c_s \|\varphi^0\|_{s,\infty} \lambda^{\sigma(s-1/2)}, \end{aligned}$$

and finally

$$\|\pi_K \psi^n\| \le c_s \lambda^{\sigma(s-1/2)} \|\varphi^0\|_{s,\infty}. \tag{6.10}$$

Note that c_s only depends on V, γ, ν and s.
Moreover, by (6.1),we have, for $\lambda \in (0, \lambda_0)$, $n \le \exp(c\lambda^{-\sigma}/2)$ and $0 \le k \le K = \lambda^{-\sigma}$,

$$(1+k)^s \big||\psi^n|_k - |\psi^0|_k\big| \le C \exp(-c\lambda^{-\sigma}/2)(1+\lambda^{-\sigma})^s \|\varphi^0\|,$$

where C depends only on V. After a possible increase of c_s, we can assume that for all $\lambda \in (0, \lambda_0)$ and all $n \le \exp(c\lambda^{-\sigma}/2)$,

$$\sup_{0\le k\le \lambda^{-\sigma}} \Big((1+k)^s \big||\psi^n|_k - |\psi^0|_k\big|\Big) \le c_s \exp(-c\lambda^{-\sigma}/4) \|\varphi^0\|. \tag{6.11}$$

This implies that for all $n \le \exp(c\lambda^{-\sigma}/2)$ and all k such that $0 \le k \le \lambda^{-\sigma}$, we have after a possible increase of c_s,

$$(1+k)^s |\psi^n|_k \le c_s \|\varphi^0\|_{s,\infty}. \tag{6.12}$$

On one hand, we have with (6.10) and after another increase of the constant c_s, for all $n \leq \exp(c\lambda^{-\sigma})$ and all $k \leq \lambda^{-\sigma}$,

$$\|\pi_K \psi^n\| \, (1+k)^{s'} \leq c_s \lambda^{\sigma(s-s'-1/2)} \|\varphi^0\|_{s,\infty} ,$$

and, since $\lambda_0 \leq 1$, for such k and n, we get

$$\|\pi_K \psi^n\| \, (1+k)^{s'} \leq c_s \|\varphi^0\|_{s,\infty} . \tag{6.13}$$

On the other hand, with Theorem 2.2 and Lemma 6.2, we get for all $n \in \mathbb{N}$,

$$\|(Q(\lambda)^* - \mathrm{Id})(\mathrm{Id} - \pi_K)\psi^n\|_{s',\infty} \leq C\lambda^{1/2} \|(\mathrm{Id} - \pi_K)\psi^n\|_{s',\infty} ,$$

where C depends only on V and s'. With the inequality (6.12), this yields, after a possible increase of the constant c_s,

$$\|(Q(\lambda)^* - \mathrm{Id})(\mathrm{Id} - \pi_K)\psi^n\|_{s',\infty} \leq c_s \lambda^{1/2} \|\varphi^0\|_{s,\infty} . \tag{6.14}$$

Hence, since for all $k \leq \lambda^{-\sigma}$ and all $n \leq \exp(c\lambda^{-\sigma}/2)$,

$$\begin{array}{rcl} \big|\, |\varphi^n|_k - |\psi^n|_k \,\big| & \leq & |\varphi^n - \psi^n|_k \\ & \leq & |(Q(\lambda)^* - \mathrm{Id})(\mathrm{Id} - \pi_K)\psi^n|_k + |(Q(\lambda)^* - \mathrm{Id})\pi_K \psi^n|_k , \end{array}$$

we derive, with (6.13) and (6.14), Lemma 6.1 and Theorem 2.2, that for such n and k,

$$\begin{array}{rl} & (1+k)^{s'} \big|\, |\varphi^n|_k - |\psi^n|_k \,\big| \\ \leq & c_s \lambda^{1/2} \|\varphi^0\|_{s,\infty} + C_{\rho_V/5} \|Q(\lambda)^* - \mathrm{Id}\|_{\rho_V/5} \|\pi_K \psi^n\| \, (1+k)^{s'} \\ \leq & c_s \lambda^{1/2} \|\pi_K \psi^n\| , \end{array}$$

after a possible increase of the constant c_s.
In addition to this last inequality and (6.11), the fact that for all $k \in \mathbb{N}$,

$$(1+k)^{s'} \Big| |\varphi^0|_k - |\psi^0|_k \Big| \leq c_s \lambda^{1/2} \|\varphi^0\|_{s,\infty}$$

which is a consequence of Theorem 2.2 and Lemma 6.2, ensures by triangle inequality, that for all $n \leq \exp(c\lambda^{-\sigma}/2)$ and $k \leq \lambda^{-\sigma}$,

$$\begin{array}{rl} & (1+k)^{s'} \big|\, |\varphi^n|_k - |\varphi^0|_k \,\big| \\ \leq & (1+k)^{s'} \big|\, |\varphi^n|_k - |\psi^n|_k \,\big| + (1+k)^{s'} \big|\, |\psi^n|_k - |\psi^0|_k \,\big| + (1+k)^{s'} \big|\, |\psi^0|_k - |\varphi^0|_k \,\big| \\ \leq & c_s \lambda^{1/2} \|\varphi^0\|_{s,\infty} , \end{array}$$

after a possible increase of the constant c_s, still depending only on V, ρ_V, γ, ν and s. This proves (2.13) and hence (ii). ∎

7 Appendix

Proof of Lemma 4.3. We consider the differential equation

$$\left\{ \begin{array}{rcl} \mathsf{q}'(t) & = & f(t, \mathsf{q}(t)) \\ \mathsf{q}(0) & = & 1 \end{array} \right.$$

with

$$f(t,Y)=\frac{\mathsf{s}_0 C_\delta Y}{1-C_\delta^2\big(\kappa(e^{2hM_V}t-1)+(Y^2-1)\big)}$$

(recall that $\mathsf{s}_0=M_V\kappa h$). This equation has a unique analytical solution: there exists a number $R>0$ such that for $t\in(-R,R)$, $\mathsf{q}(t)$ expands in power series of t (see for instance [8]). We can assume that R is maximal in this sense. Let

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

For $0\le t\le T$ we have $\kappa C_\delta^2(e^{2hM_Vt}-1)\le\frac14$ and if $1\le Y\le 1+D$, then $C_\delta^2(Y^2-1)\le\frac14$. Therefore,

$$\begin{cases}0\le t\le T\\ 0\le Y-1\le D\end{cases}\implies 0<f(t,Y)\le 2\mathsf{s}_0C_\delta(D+1).\tag{7.1}$$

This implies that q is an increasing function of t as long as $t\in(0,T)$ and $\mathsf{q}(t)\le D+1$. Notice that, for $t\ge 0$, we have $0<\mathsf{q}(t)\le 1$.
Moreover, the fact that $K\ge K_0\ge 1$ (see Lemma 4.3) implies that $\frac{1}{\kappa}\le 4$ and hence we have

$$T=\frac{2}{hM_V}\ln\Big(1+\frac{1}{4\kappa C_\delta^2}\Big)\ge\frac{1}{4hM_V\kappa C_\delta^2}.\tag{7.2}$$

If for all $t\in(0,R)$, $1<\mathsf{q}(t)<1+D$, we must have in view of (7.1), $T<R$. To the contrary, there exists t_D^* in $(0,R)$ such that $\mathsf{q}(t_D^*)=1+D$. We can therefore choose $t_D^*\in(0,R)$ in such a way that for all $t\in(0,t_D^*)$, $1<\mathsf{q}(t)<1+D$.
Assume that $t_D^*\le T$, then

$$y(t_D^*)-y(0)=D\le\int_0^{t_D^*}f(u,y(u))\mathrm{d}u\le 2\mathsf{s}_0C_\delta(D+1)t_D^*$$

using (7.1) Hence we have

$$\begin{aligned}t_D^* &\ge\ =\frac{D}{2\mathsf{s}_0C_\delta(D+1)}\\ &\ge \frac{(1+\frac{1}{4C_\delta^2})^{\frac12}-1}{(1+\frac{1}{4C_\delta^2})^{\frac12}}\frac{1}{2\kappa hM_VC_\delta}\\ &\ge \frac{1}{16C_\delta^2\Big(1+\frac{1}{4C_\delta^2}\Big)}\frac{1}{\kappa hM_VC_\delta}\\ &\ge \frac{1}{4hM_V\kappa C_\delta^2}\frac{1}{5C_\delta}.\end{aligned}$$

Hence, we have

$$R>t_D^*\ge\frac{1}{20hM_V\kappa C_\delta^3}.\tag{7.3}$$

To the contrary, if $t_D^* \geq T$ then we have using (7.2)

$$R > T \geq \frac{1}{4hM_V \kappa C_\delta^2}.$$

As $C_\delta^{-1} \leq 1$, this implies that (7.3) holds in any case. This determines the value of $r < R$ in the Lemma. Now as $t \mapsto \mathsf{q}(t)$ is an increasing positive function, so is $t \mapsto \mathsf{q}'(t) = f(t, \mathsf{q}(t))$.
With the previous notations, in any case, we have with (7.1) that for all $t \in (-r, r)$

$$\mathsf{q}'(t) \leq \frac{\kappa h M_V C_\delta (D+1)}{1 - \frac{1}{4} - \frac{1}{4}} \leq \sqrt{5} \kappa h M_V C_\delta.$$

We have already seen that for all $t \in (0, r)$, $1 \leq \mathsf{q}(t) \leq D + 1 \leq \frac{\sqrt{5}}{2}$. And it follows from the estimation on q' that

$$\mathsf{q}(-r) = 1 - \int_{-r}^{0} \mathsf{q}'(s) \mathrm{d}s \geq 1 - r\sqrt{5}\kappa h M_V C_\delta > 0.8 \; .$$

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

Acknowledgments

The authors are glad to thank François Castella, Philippe Chartier, Nicolas Lerner and Christian Lubich for their help and comments about this work.

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