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Long time behavior of splitting methods applied to the linear Schrödinger equation

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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 analytical size of the potential, we show the conservation over exponentially long time of the energies associated with the double eigenvalues of the Laplace operator for asymptotically large modes. The result relies on a normal form theorem whose proof uses standard techniques of classical perturbations theory, extended here to an infinite dimensional context. ***To cite this article: G. Dujardin, E. Faou, C. R. Acad. Sci. Paris, Ser. I 344 (2007).***

Résumé

Comportement en temps long des méthodes de splitting appliquées à l'équation de Schrödinger linéaire. Nous considérons la semi-discrétisation en temps de l'équation de Schrödinger linéaire sur un tore de dimension un par une méthode de splitting. Sous une condition de non-résonance sur le pas de temps et sous l'hypothèse que le potentiel est petit et analytique, nous montrons la conservation des énergies associées aux valeurs propres doubles du Laplacien sur des temps exponentiellement longs et pour des modes asymptotiquement grands. Le résultat repose sur un théorème de forme normale dont la preuve utilise la théorie classique des perturbations, appliquée ici à un problème de dimension infinie. ***Pour citer cet article : G. Dujardin, E. Faou, C. R. Acad. Sci. Paris, Ser. I 344 (2007).***

1. Introduction

We consider the linear Schrödinger equation

$$\mathrm{i}\frac{\partial\varphi}{\partial t}(x,t) = -\frac{\partial^2\varphi}{\partial x^2}(x,t) + V(x)\varphi(x,t), \quad \text{with } \varphi(x,0) = \varphi^0(x), \tag{1}$$

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where $\varphi(x,t)$ is a complex function depending on the space variable $x \in \mathbb{T} := \mathbb{R}/2\pi\mathbb{Z}$ and the time $t \geqslant 0$. The potential $V(x)$ is a real function and the function φ^0 is the initial value at $t = 0$. For a given time step $h > 0$, we consider the approximation scheme

$$\varphi(h) \simeq \exp(\mathrm{i}h\Delta)\exp(-\mathrm{i}hV)\varphi(0) \tag{2}$$

where by definition, $\exp(\mathrm{i}h\Delta)\varphi$ and $\exp(-\mathrm{i}hV)\varphi$ are the solutions at the time $t = h$ of the equations

$$\mathrm{i}\frac{\partial\psi(t)}{\partial t} = -\Delta\psi(t), \quad \text{with} \quad \psi(0) = \varphi, \quad \text{and} \quad \mathrm{i}\frac{\partial\psi(t)}{\partial t} = V\psi(t), \quad \text{with } \psi(0) = \varphi$$

respectively. If the potential is smooth enough, it can be shown that the approximation (2) is a first order approximation of the solution of (1), see [4] and [1] (where the non-linear case is studied). Note moreover that the scheme (2) conserves the L^2 norm. As the problem (1) is set on an infinite dimensional space of functions, the long time behavior of this method cannot be analyzed using classical backward error analysis (see for instance [3,5]) and the Baker–Campbell–Hausdorff formula.

To study the long time behavior of the numerical scheme (2), we consider the family of Hamiltonians

$$H(\lambda) = -\Delta + \lambda V, \quad \lambda \in \mathbb{R}, \tag{3}$$

with λ sufficiently small and with an analytic potential V. We denote by

$$L(\lambda) = \exp(\mathrm{i}h\Delta)\exp(-\mathrm{i}h\lambda V), \quad \lambda \in \mathbb{R}, \tag{4}$$

the corresponding family of propagators. The Hamiltonian $H(\lambda)$ is thus viewed as an analytic perturbation of the Hamiltonian $H(0) = -\Delta$ which is completely integrable in the sense where the dynamics can be reduced to an (infinite) collection of periodic systems in terms of Fourier coefficients of the solution.

We use the following non-resonance condition on the stepsize: There exist $\gamma > 0$ and $\nu > 1$ such that

$$\forall k \in \mathbb{Z},\ k \neq 0, \quad \left|\frac{1 - \mathrm{e}^{\mathrm{i}hk}}{h}\right| \geqslant \gamma|k|^{-\nu}. \tag{5}$$

It can be shown that the set of stepsizes $h \in (0, h_0)$ that do not satisfy (5) has a Lebesgue measure $\mathcal{O}(h_0^{r+1})$ for $r > 1$ when $h_0 > 0$ is close to 0 (see [3,6]).

2. Statement of the results

In all this Note, we identify a function $\psi(x)$ and its Fourier transform on $\mathbb{T}$. This means that we write ψ_n the nth Fourier coefficient of ψ for all $n \in \mathbb{Z}$, and identify the collection $(\psi_n)_{n\in\mathbb{Z}}$ with the function ψ itself. We 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 $\psi = (\psi_n)_{n\in\mathbb{Z}} \in \mathbb{C}^{\mathbb{Z}}$, the product $\varphi = S\psi$ is defined by the sequence $\varphi = (\varphi_n)_{n\in\mathbb{Z}}$ of $\mathbb{C}^{\mathbb{Z}}$ with coefficients $\varphi_n := \sum_{k\in\mathbb{Z}} S_{nk}\psi_k$, provided the summation makes sense. For two operators A and B, the product AB is the operator whose coefficients are given formally by the relation

$$\forall (i,j) \in \mathbb{Z}^2, \quad (AB)_{ij} = \sum_{k\in\mathbb{Z}} A_{ik}B_{kj}. \tag{6}$$

We define the analytic norm for functions

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

for a given positive number ρ. We make the assumption that there exists $\rho_V > 0$ such that $\|V\|_{\rho_V} < \infty$. In the following, for a function φ we use the notation

$$|\varphi|_0^2 = |\varphi_0|^2 \quad \text{and} \quad \forall k \in \mathbb{Z}\backslash\{0\}, \quad |\varphi|_k^2 = |\varphi_k|^2 + |\varphi_{-k}|^2 \tag{7}$$

to denote the energies associated with the double eigenvalues $-k^2$ of the Laplace operator. Moreover, for $s > 0$ we introduce the norm

$$\|\varphi\|_{s,\infty} = \sup_{k\geqslant 0}\big((1+k)^s|\varphi|_k\big). \tag{8}$$

We can prove the following result concerning the long time behavior of the numerical solution provided by the splitting method (2):

Theorem 2.1. *For $n \in \mathbb{N}$, we set $\varphi^n = L(\lambda)^n \varphi^0$. There exist positive constants C, c, λ_0, and σ depending only on V, γ and ν such that for all $h \in (0,1)$ satisfying the non-resonance condition* (5)*, all $\lambda \in (0, \lambda_0)$, $n \leqslant \exp(c\lambda^{-\sigma}/2)$, and $\varphi^0 \in L^2(\mathbb{T})$,*

$$\forall k \in \mathbb{N},\ k \leqslant \lambda^{-\sigma}, \quad \big| |\varphi^n|_k - |\varphi^0|_k \big| \leqslant C\lambda^{1/2} \|\varphi^0\|. \tag{9}$$

Moreover, the two following propositions hold true:

(i) *For all $s > 1/2$ and all s' such that $s - s' \geqslant 1/2$, there exists a constant c_s depending only on V, γ, ν and s, such that for all $h \in (0,1)$ satisfying* (5)*, all $\lambda \in (0,\lambda_0)$, $n \leqslant \exp(c\lambda^{-\sigma}/2)$, and φ^0 with $\|\varphi^0\|_{s,\infty} < +\infty$, we have*

$$\sup_{0 \leqslant k \leqslant \lambda^{-\sigma}} \big((1+k)^{s'} \big| |\varphi^n|_k - |\varphi^0|_k \big| \big) \leqslant c_s \lambda^{1/2} \|\varphi^0\|_{s,\infty}. \tag{10}$$

(ii) *For all $\rho \in (0, \rho_V/5)$, there exist positive constants μ_0 and C_ρ (depending only on V, γ, ν and ρ) such that for all $h \in (0,1)$ satisfying* (5)*, all $\lambda \in (0,\lambda_0)$, $n \leqslant \exp(c\lambda^{-\sigma}/2)$, $\mu \in (0,\mu_0)$ and φ^0 with $\|\varphi^0\|_\rho < \infty$,*

$$\sup_{0 \leqslant k \leqslant \lambda^{-\sigma}} \big(\mathrm{e}^{\mu k} \big| |\varphi^n|_k - |\varphi^0|_k \big| \big) \leqslant C_\rho \lambda^{1/2} \|\varphi^0\|_\rho. \tag{11}$$

The inequality (9) expresses the fact that the oscillatory energies $|\varphi|_k$ are conserved over very long time for asymptotically large modes k. The inequalities (10) and (11) give more precise estimates in the case where the initial condition has more regularity.

3. Sketch of proof

The proof of the theorem relies on a normal form result given in [2]. We explain here the main ideas. For an operator S and for $\rho \in \mathbb{R}^+$, we define the norm

$$\|S\|_\rho = \sup_{k,\ell \in \mathbb{Z}} \big(\mathrm{e}^{\rho|k-\ell|} |S_{k\ell}| \big) \tag{12}$$

and we set $\mathcal{A}_\rho$ the space of operators S with finite norm $\|S\|_\rho < \infty$. We define moreover the *X-shaped* operators as the elements $X \in \mathcal{A}_\rho$ for which we have $X_{k\ell} \neq 0 \Longrightarrow |k| = |\ell|$. For a given $K > 0$ we define the set of indices

$$I_K = \big\{ (k,\ell) \in \mathbb{Z} \mid |k| \leqslant K \text{ or } |\ell| \leqslant K \big\}. \tag{13}$$

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

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

It is worth noticing that under the action of a given almost X-shaped operator, all the spaces $\{\varphi \mid \varphi_j \neq 0 \Longrightarrow j = \pm k\}$, $|k| \leqslant K$, are invariant, as well as the space $\{\varphi \mid \varphi_j \neq 0 \Longrightarrow |j| > K\}$.

In [2] we prove the following result: There exist positive constants c, λ_0 and σ depending only on V, γ and ν and families of operators $Q(\lambda)$, $\Sigma(\lambda)$ and $R(\lambda)$ analytic in λ for $|\lambda| < \lambda_0$ such that for $\lambda \in (0,\lambda_0)$ and all $h \in (0,1)$ satisfying (5), we can write

$$Q(\lambda) L(\lambda) Q(\lambda)^* = \Sigma(\lambda) + R(\lambda)$$

with the estimate

$$\big\| R(\lambda) \big\|_{\rho_V/5} \leqslant \exp(-c\lambda^{-\sigma}). \tag{14}$$

Moreover, the operators $Q(\lambda)$ and $\Sigma(\lambda)$ are unitary for all λ, and satisfy for $\lambda \in (0,\lambda_0)$

$$\big\| Q(\lambda) - \mathrm{Id} \big\|_{\rho_V/4} \leqslant \lambda^{1/2} \quad \text{and} \quad \big\| \Sigma(\lambda) - \mathrm{e}^{\mathrm{i}h\Delta} \big\|_{\rho_V/4} \leqslant h\lambda^{1/2}.$$

Eventually, we have

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

that is, $\Sigma(\lambda)$ is a unitary almost X-shaped operator.

Roughly speaking, this 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 dynamics for each modes $\pm k$. This is valid for asymptotically large modes $|k| \leqslant \lambda^{-\sigma}$. More precisely, if φ is a function and if $\psi = \Sigma(\lambda)\varphi$, we have for $|k| \leqslant \lambda^{-\sigma}$,

$$\begin{pmatrix} \psi_k \\ \psi_{-k} \end{pmatrix} = \begin{pmatrix} a_k(\lambda) & b_k(\lambda) \\ c_k(\lambda) & d_k(\lambda) \end{pmatrix} \begin{pmatrix} \varphi_k \\ \varphi_{-k} \end{pmatrix} \tag{15}$$

where the 2×2 matrix in this relation is close to the diagonal matrix with entries $\mathrm{e}^{-\mathrm{i}hk^2}$, and is unitary. This implies that we have for $|k| \leqslant \lambda^{-\sigma}$, $|\psi_k|^2 + |\psi_{-k}|^2 = |\varphi_k|^2 + |\varphi_{-k}|^2$. Combining this conservation law for the action of $\Sigma(\lambda)$ with the exponential estimate (14) allows us to obtain the long time bounds of Theorem 2.1.

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