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QUALITATIVE BEHAVIOR OF SPLITTING METHODS FOR THE LINEAR SCHRÖDINGER EQUATION IN MOLECULAR DYNAMICS

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Abstract. We present a normal form theorem for the propagator of a splitting method applied to a linear Schrödinger equation. This result allows us to derive conservation properties for the numerical solutions provided by the method. As a conclusion, we show numerical experiments illustrating our results.

Contents

1. Introduction

In the context of molecular dynamics, an important issue is to be able to compute "good" numerical approximations over long time of the solutions of the autonomous linear Schrödinger equation with a linear multiplicative potential. This kind of Schrödinger equation reads

$$\begin{cases} i\dfrac{\partial}{\partial t}\psi(t,x) &=& H\psi(t,x) \\ \psi(0,x) &=& \psi_0(x) \end{cases} \tag{1.1}$$

where ψ denotes the unknown complex wave function depending on the time variable $t \in \mathbb{R}$ and the space variable $x \in \mathbb{R}^{Nd}$ (where $d \in \{1,2,3\}$ is the space dimension and $N \in \mathbb{N}^*$ is the number of particles); ψ_0 stands for the known wave function of the system of particles in the initial state. Moreover, the hamiltonian H is for physical reasons the sum of a kinetic term T and a potential term V that read

$$T = -\sum_{k=1}^{N} \frac{1}{2\,m_k}\Delta_{x_k} \qquad \text{and} \qquad V = V(x)$$

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where for all $k \in \{1, \ldots, N\}$, $m_k > 0$ denotes the mass of the kth particle and V is (a multiplication operator by) a real function of x.

Such a decomposition of the hamiltonian of the Cauchy problem (1.1) leads us to consider the use of splitting methods to compute numerical solutions. Our goal is to describe and explain, thanks to the study of a simplified model problem of type (1.1), the behavior of the numerical solutions computed by splitting methods; a specific emphasis will be put on the conservation of the space regularity of these solutions.

We begin by a presentation of the hypothesis we make throughout this paper and a description of the numerical splitting methods we consider. Then, we give a geometric theorem of normal form for the propagator of these splitting methods that we prove in [5]. This theorem allows us to state a result describing the long time behavior of the numerical solutions. As a conclusion, we show some numerical experiments that illustrate our results.

2. Notations and hypothesis

The context of our work is the following : we consider one particule ($N = 1$) of mass $m_1 = 1/2$, in one space dimension ($d = 1$). We do consider a periodic problem : the initial data ψ_0 depends on $x \in \mathbb{T}$ (where $\mathbb{T}$ denotes the one dimensional torus) and the wave function ψ is also periodic in space, depending on $x \in \mathbb{T}$ and $t \in \mathbb{R}$.

In order to compute numerical solutions of the Cauchy problem (1.1), we consider splitting methods that use the propagators of the following Cauchy problems :

$$\left\{ \begin{array}{rcll} i\partial_t\varphi(t,x) & = & V(x)\varphi(t,x) & (t,x) \in \mathbb{R}\times\mathbb{T} \\ \varphi(0,x) & = & \varphi_0(x) & x \in \mathbb{T} \end{array} \right. \tag{2.1}$$

and

$$\left\{ \begin{array}{rcll} i\partial_t\varphi(t,x) & = & -\Delta\varphi(t,x) & (t,x) \in \mathbb{R}\times\mathbb{T} \\ \varphi(0,x) & = & \varphi_0(x) & x \in \mathbb{T} \end{array} \right. . \tag{2.2}$$

For a time step $h > 0$, $e^{-ihV}\varphi_0$ denotes the solution at time h of the problem (2.1) and $e^{ih\Delta}\varphi_0$ denotes the solution at time h of the problem (2.2). The computation of $e^{-ihV}\varphi_0$ is numerically made by solving an ordinary differential equation on a grid, while the computation of $e^{ih\Delta}\varphi_0$ is carried out by a fast Fourier transform.

Let us consider the Lie splitting method definied by the propagator

$$L_\lambda = e^{ih\Delta}e^{-ih\lambda V} \tag{2.3}$$

where $\lambda \in \mathbb{R}$ is a parameter that will allow us to consider that V is "small" when compared to the first positive eigenvalue of $-\Delta$, in such a way that the propagator L_λ will be considered as a perturbation of the free Schrödinger propagator $e^{ih\Delta} = L_0$. Notice that most of our results extend for example to the Lie splitting method $L^{(1)} = e^{-ihV}e^{ih\Delta}$ and to the Strang splitting methods $L^{(2,1)} = e^{i\frac{h}{2}\Delta}e^{-ihV}e^{i\frac{h}{2}\Delta}$ and $L^{(2,2)} = e^{-i\frac{h}{2}V}e^{ih\Delta}e^{-i\frac{h}{2}V}$.

In order to study the conservation of the regularity of the numerical solutions computed by the splitting method defined by the propagator (2.3), we assume that V is a 2π-periodic function that is analytic in an 2π-periodic open set of the complex plane containing the set $[0, 2\pi] + i[-\rho_V, \rho_V]$ for a given $\rho_V > 0$. Hence, if for all $n \in \mathbb{Z}$, V_n denotes the nth Fourier coefficient of V, then for all $n \in \mathbb{Z}$, we have $|V_n| \leq M_V e^{-\rho_V|n|}$.

Throughout this paper, we identify $L^2(\mathbb{T})$ and $l^2(\mathbb{Z})$ by the Fourier coefficients; we identify the subspaces of $L^2(\mathbb{T})$ and those of $l^2(\mathbb{Z})$; we also identify operators defined on a subspace of $L^2(\mathbb{T})$ and operators defined on a subspace of $l^2(\mathbb{Z})$. For such an operator A, we define the quantities

$$\|A\|_\mu = \sup\{|A_{n,m}|e^{+\mu|n-m|} \quad | \quad (n,m) \in \mathbb{Z}^2\} \qquad \text{for } \mu \in \mathbb{R}^+.$$

We denote by $\mathcal{A}_\mu$ the space of operators A such that $\|A\|_\mu < \infty$. Moreover, for $K > 0$, we discriminate among operators of $\mathcal{A}_\mu$ those who are K-*almost-cross* in the sense that they do satisfy

$$\forall (i,j) \in \mathbb{Z}^2 \text{ such that } |i| \le K \text{ or } |j| \le K, \qquad \big(A_{ij} \neq 0 \Rightarrow |i| = |j|\big).$$

We denote by $\mathcal{X}_\mu^K$ the subspace of $\mathcal{A}_\mu$ containing all the K-almost-cross operators.

For the functions of $L^1(\mathbb{T})$, we define the following quantities

$$\begin{aligned} \|\varphi\| &= \Big(\sum_{k\in\mathbb{Z}} |\varphi_k|^2\Big)^{\frac{1}{2}}, \\ \|\varphi\|_{s,\infty} &= \sup_{k\ge 0}\Big((1+k)^s(|\varphi_k|^2 + |\varphi_{-k}|^2)^{1/2}\Big), \qquad s \in \mathbb{R}^+, \\ \|\varphi\|_\rho &= \sup_{n\in\mathbb{Z}} |\varphi_k| e^{+\rho|k|}, \qquad \rho \in \mathbb{R}^+. \end{aligned}$$

At last, in order to state our results, we need the following non-resonance condition on the time step $h > 0$ (cf [7, 12]) : there exists $\gamma > 0$ and $\nu > 1$ such that

$$\forall\, k \in \mathbb{Z}, \quad k \neq 0, \quad \left|\frac{1 - e^{ihk}}{h}\right| \ge \gamma |k|^{-\nu}. \tag{2.4}$$

Notice that, for $h_0 > 0$ close to zero, the set of the $h \in (0, h_0)$ that do not satisfy (2.4) has a Lebesgue measure $\mathcal{O}(h_0^{r+1})$ for an $r > 1$ (cf [7, 12]).

3. A normal form result for the splitting propagator

The normal form theorem for the splitting propagator that we prove in [5] is the following :

Theorem 3.1. *Consider V and $(L_\lambda)_{\lambda\in\mathbb{R}}$ satisfying the hypothesis above. Assume $\gamma > 0$ and $\nu > 1$ are positive real numbers. There exists three positive constants λ_0, c and σ such that for all $h \in (0, 1)$ satisfying* (2.4)*, there exists families of operators $Q(\lambda)$ and $\Sigma(\lambda)$ that are analytical with respect to λ for $|\lambda| < \lambda_0$ such that for all $\lambda \in (0, \lambda_0)$,*

$$Q(\lambda) \in \mathcal{A}_{\rho_V/4} \quad \textit{and} \quad \Sigma(\lambda) \in \mathcal{X}^K_{\rho_V/4} \quad \textit{with} \quad K = \lambda^{-\sigma} \tag{3.1}$$

$$\|Q(\lambda) - \mathrm{Id}\|_{\rho_V/4} \le \lambda^{1/2} \quad \textit{and} \quad \|\Sigma(\lambda) - e^{ih\Delta}\|_{\rho_V/4} \le h\lambda^{1/2}, \tag{3.2}$$

and

$$Q(\lambda)^* Q(\lambda) = \mathrm{Id}, \quad \textit{and} \quad \Sigma(\lambda)^*\Sigma(\lambda) = \mathrm{Id}, \tag{3.3}$$

and such that the following relation holds

$$Q(\lambda) L_\lambda Q(\lambda)^* = \Sigma(\lambda) + R(\lambda), \tag{3.4}$$

where the remainder $R(\lambda)$ satisfies, for $\lambda \in (0, \lambda_0)$,

$$\|R(\lambda)\|_{\rho_V/5} \le \exp(-c\lambda^{-\sigma}). \tag{3.5}$$

This result shows that, after a unitary change of variable close to identity in an analytical norm, the dynamics generated by the splitting propagator reduces (up to exponentially small terms with respect to λ) to the action of $\Sigma(\lambda)$. Moreover, the action of this operator itself reduces to a dynamics made of small symplectic 2×2 systems by pairs of modes $\pm k$ for asymptotically large modes ($|k| \le \lambda^{-\sigma}$)

with respect to λ, since it is unitary and K-almost-cross (see (3.1), (3.2) et (3.3)). As a consequence, if we denote by

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

the *coupled energies* at modes $\pm k$, then we have for $\varphi, \psi \in L^2$ such that $\psi = \Sigma(\lambda)\varphi$,

$$\forall k \in \mathbb{Z} \quad \text{s.t.} \quad |k| \leq \lambda^{-\sigma}, \quad |\varphi|_k = |\psi|_k. \tag{3.6}$$

The concurrence of the conservation property (3.6) and of the analytical estimations (3.4) and (3.5) allows us to prove conservation properties over long time for numerical solutions of (1.1) computed by iterations of L_λ.

4. Behavior over long time of the numerical solutions provided by the splitting method

With the help of the normal form Theorem 3.1 for the propagator of the splitting method (2.3), we show in [5] that the following result dealing with the long time behavior of the numerical solutions of (1.1) computed by the splitting method (2.3) holds :

Corollary 4.1. *Under the hypothesis of Theorem 3.1, if we denote for all* $n \in \mathbb{N}$, $\varphi^n = L_\lambda^n \varphi^0$, *then*
(i) *There exists a positive constant* C *depending only on* V, γ *and* ν *such that for all* $h \in (0,1)$ *satisfying* (2.4), *all* $\lambda \in (0, \lambda_0)$, *all* $n \leq \exp(c\lambda^{-\sigma}/2)$, *and all* $\varphi^0 \in L^2(\mathbb{T})$, *we have*

$$\forall\, k \in \mathbb{N}, \quad k \leq \lambda^{-\sigma}, \quad \big|\, |\varphi^n|_k - |\varphi^0|_k \,\big| \leq C\lambda^{1/2} \|\varphi^0\| \,. \tag{4.1}$$

(ii) *Assume* $s > 1/2$ *and* $s' \in \mathbb{R}$ *are such that* $s - s' \geq 1/2$, *then there exists a constant* $c_s > 0$ *depending only on* V, γ, ν *and* s *such that for all* $h \in (0,1)$ *satisfying* (2.4), *all* $\lambda \in (0, \lambda_0)$, *all* $n \leq \exp(c\lambda^{-\sigma}/2)$, *and all* φ^0 *such that* $\|\varphi^0\|_{s,\infty} < +\infty$, *we have*

$$\sup_{0 \leq k \leq \lambda^{-\sigma}} \Big((1+k)^{s'} \,\big|\, |\varphi^n|_k - |\varphi^0|_k \,\big| \Big) \leq c_s \lambda^{1/2} \|\varphi^0\|_{s,\infty} \,. \tag{4.2}$$

(iii) *For* $\rho \in (0, \rho_V/5)$, *there exists positive contants* μ_0 *and* C *depending only on* V, γ, ν *and* ρ *such that for all* $h \in (0,1)$ *satisfying* (2.4), *all* $\lambda \in (0, \lambda_0)$, *all* $n \leq \exp(c\lambda^{-\sigma}/2)$, *all* $\mu \in (0, \mu_0)$ *and all* φ^0 *such that* $\|\varphi\|_\rho < \infty$, *we have*

$$\sup_{0 \leq k \leq \lambda^{-\sigma}} \Big(e^{\mu k} \,\big|\, |\varphi^n|_k - |\varphi^0|_k \,\big| \Big) \leq C \lambda^{1/2} \|\varphi^0\|_\rho \,. \tag{4.3}$$

The next section is aimed at illustrating this result dealing with the conservation of regularity for the numerical solutions computed by the splitting method. In particular, we will illustrate the (i) of Corollary 4.1.

5. Numerical experiments

In this section, we show the numerical results obtained with the numerical splitting method L_λ defined in (2.3). For our computations, we use the following data :

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

We use two different time steps for these computations :

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

The first time step satisfies the non-resonance condition (2.4), while the second one obviously is resonant.

On the first figure, we plot the 5 first coupled energies computed with $N = 2^7 + 1 = 129$ Fourier modes; we do show the results after 10^6 iterations computed with $\lambda = 0.1$. The numerical results illustrate that, if the non-resonance condition is satisfied, then the properties of conservation of regularity for the numerical solution predicted by Corollary 4.1 do hold. On the other hand, for a resonant time step, these properties do not hold anymore.

On the second figure, we plot all the coupled energies computed with $N = 2^9 + 1 = 513$ Fourier modes for 10^5 iterations with $\lambda = 0.01$. For the resonant time step, we see a huge increase of coupled energies for some high order modes (recall that the L^2-norm is preserved), while for the non-resonant time step, all of them are well preserved, as predicted by Corollary 4.1.

On the third figure, we plot the quantities $f(n) = \left(\sum_{k=0}^{N} |\varphi^n|_k^2 e^{+2\rho k}\right)^{1/2}$ divided by $f(0)$, with $N = 2^6 = 64$ and $\rho = 1$, in function of time. The computations are carried out with $\tilde{N} = 2^{12}+1 = 4097$ modes and $\lambda = 0.01$. The final time is $T = 500$ and the time steps are again the previous ones. For the resonant time step, we see that the approximated analytical norm $f(n)$ increases exponentially, and that this is not the case for the non-resonant time step. This is an illustration of estimation (4.3) of Corollary 4.1.

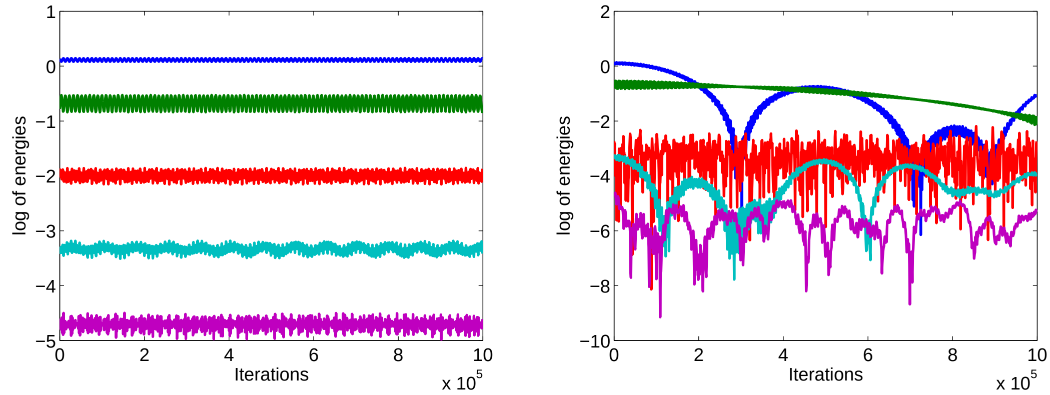

FIGURE 1. Coupled energies defined above for the first 5 modes of the numerical solution in logarithmic scale, $\lambda = 0.1$. Non-resonant (left) and resonant (right) time steps.

With these numerical experiments, we illustrate the fact that the conservation property (4.1) in Corollary 4.1 holds true for non-resonant time steps (that is to say for time steps satisfying (2.4)), while this conservation property may be violated for resonant time steps.

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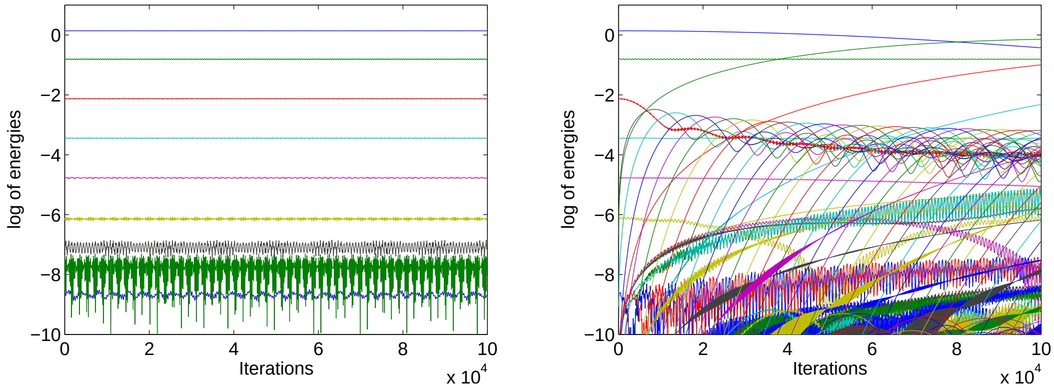

FIGURE 2. Coupled energies defined above in logarithmic scale, $\lambda = 0.01$. Non-resonant (left) and resonant (right) time steps.

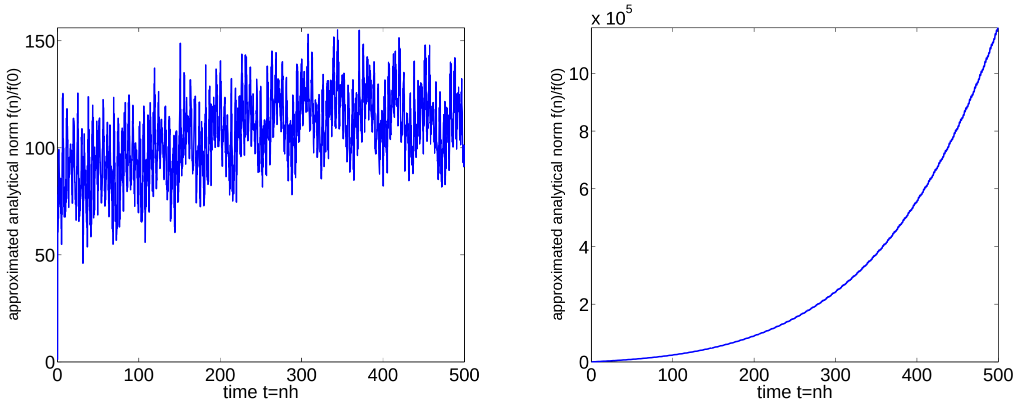

FIGURE 3. Approximations of the analytical norm of the numerical solution with $\lambda = 0.01$. Non-resonant (left) and resonant (right) time steps.

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