Lagrange–Schwarz Waveform Relaxation domain decomposition methods for linear and nonlinear quantum wave problems[☆]

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A B S T R A C T

A Schwarz Waveform Relaxation (SWR) algorithm is proposed to solve by Domain Decomposition Method (DDM) linear and nonlinear Schrödinger equations. The symbols of the transparent fractional transmission operators involved in Optimized Schwarz Waveform Relaxation (OSWR) algorithms are approximated by low order Lagrange polynomials to derive Lagrange–Schwarz Waveform Relaxation (LSWR) algorithms based on local transmission operators. The LSWR methods are numerically shown to be computationally efficient, leading to convergence rates almost similar to OSWR techniques.

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1. Introduction and methodology

Let us consider the following initial–boundary-value problem: find the complex-valued wavefunction $u(\mathbf{x}, t)$ solution to the real-time NonLinear cubic Schrödinger Equation (NLSE) [1–3] set on $\mathbb{R}^d$, $d \geqslant 1$,

$$\begin{cases} \mathrm{i}\partial_t u = -\triangle u + V(\mathbf{x})u + \kappa|u|^2 u, & \mathbf{x} \in \mathbb{R}^d,\, t > 0, \\ u(\mathbf{x}, 0) = u_0(\mathbf{x}), & \mathbf{x} \in \mathbb{R}^d, \end{cases} \quad (1)$$

with initial condition u_0, nonlinearity strength $\kappa \geqslant 0$ and smooth potential $V(\mathbf{x}) > 0$. When $\kappa = 0$, (1) refers to as the Linear Schrödinger Equation (LSE). The objective of the letter is the derivation of simple, accurate and efficient transmission conditions for SWR-DDMs. In 1d ($d = 1$), the general principle consists of approximating nonlocal fractional operators, such as $\pm\sqrt{-\mathrm{i}\partial_t + V}$, for V constant, which are involved in

OSWR transmission conditions [4] by simple low order partial differential operators. For space-dependent potentials V, OSWR methods for LSE/NLSE are derived from artificial operators $\partial_x + \Lambda^\pm(x, \partial_t)$, where $\Lambda^\pm(x, \partial_t) = \mathrm{Op}\big(\lambda^\pm(x, \tau)\big)$, with $\lambda^\pm(x, \tau) = \sigma(\Lambda^\pm)$ where τ is the covariable associated to t, through a Nirenberg factorization, and $\sigma(A)$ is the symbol of a given pseudodifferential operator A. We also introduce $\Lambda_p^\pm = \mathrm{Op}\big(\lambda_p^\pm(x, \tau)\big)$, where $\lambda_p^\pm(x, \tau) = \pm\sqrt{\tau + V(x)} = \sigma_p(\Lambda^\pm)$ is the principal symbol of $\Lambda^\pm$. We can show [5] for instance that for $|\tau| \gg 1$, $\lambda_p(x, \tau) - \lambda(x, \tau) = \mathcal{O}(\tau^{-1})$, and similar estimates can be established for $|\tau| \ll 1$. Despite the fast convergence of OSWR methods [4,6,7], their prohibitive cost in quantum wave problems is a consequence of the nonlocal character in time of the fractional operators $\Lambda^\pm$ and $\Lambda_p^\pm$ [5,8]. These operators thus require the storage at all times of the solution at the subdomain interfaces which is computationally expensive. In addition, the derivation of a stable and accurate discretization is non-trivial. This is extensively discussed for (1) in the framework of absorbing boundary condition in [9,10]. We propose in this letter to approximate $\lambda_p^\pm$ using Lagrange polynomials of degree $i \geqslant 1$ in τ, $\ell_i^\pm(x, \tau) = \sum_{k=0}^{i} a_i^\pm(x)\tau^k$ [11]. Notice that more generally, if explicit expressions of the *exact* symbol $\lambda^\pm$ are known, it is possible to apply the methodology presented in this letter directly to $\lambda^\pm$. For $i = 0$, the corresponding transmission operator is a Robin operator. The associated SWR algorithm was analyzed for the LSE in [4]. In a second stage, we reconstruct the corresponding differential operators from these polynomial symbols. The interest of the presented methodology is three-fold: (i) as the interpolation by Lagrange polynomials is performed from $\lambda_p^\pm$, we expect a fast SWR convergence [8], (ii) as the corresponding transmission operators are local differential operators, we expect a competitive computational complexity compared to OSWR methods, and finally (iii) the derivation of the Lagrange polynomial is performed from $\lambda_p^\pm$ without additional assumption on the magnitude of $|\tau|$. Then for $\tau \in (0, \tau_\infty)$ and any x, we have

$$\big\|\lambda_p^\pm(x, \cdot) - \ell_i^\pm(x, \cdot)\big\|_\infty \leqslant \frac{\tau_\infty^{i+1}}{(i+1)!}\big\|\partial_t^{(i+1)}\lambda_p^\pm(x, \cdot)\big\|_\infty.$$

Assuming that τ varies between 0^+ and τ_∞, we easily prove that, the Lagrange polynomial of degree one at $(0^+, \lambda_p^\pm(x, 0^+))$ and $(\tau_\infty, \lambda_p^\pm(x, \tau_\infty))$ reads

$$\ell_1^\pm(x, \tau) = \pm\left(\sqrt{V(x)} + \frac{\sqrt{V(x) + \tau_\infty} - \sqrt{V(x)}}{\tau_\infty}\tau\right).$$

The corresponding first-order differential operator in time is then

$$L_1^\pm(x, \partial_t) = \pm\left(\sqrt{V(x)} - i\frac{\sqrt{V(x) + \tau_\infty} - \sqrt{V(x)}}{\tau_\infty}\partial_t\right). \tag{2}$$

Denoting now by $\tau_m \in (0, \tau_\infty)$, the quadratic Lagrange polynomial at $(0^+, \lambda_p^\pm(x, 0^+))$, $(\tau_m, \lambda_p^\pm(x, \tau_m))$ and $(\tau_\infty, \lambda_p^\pm(x, \tau_\infty))$ is given by

$$\ell_2^\pm(x, \tau) = \pm\big(\sqrt{V(x)} + \alpha_{m,\infty}(x)\tau + \beta_{m,\infty}(x)\tau^2\big)$$

with

$$\alpha_{m,\infty}(x) = \frac{\tau_\infty^2\sqrt{V(x) + \tau_m} - \tau_m^2\sqrt{V(x) + \tau_\infty} + (\tau_m^2 - \tau_\infty^2)\sqrt{V(x)}}{\tau_\infty^2\tau_m - \tau_m^2\tau_\infty},$$

$$\beta_{m,\infty}(x) = \frac{\tau_m\sqrt{V(x) + \tau_\infty} - \tau_\infty\sqrt{V(x) + \tau_m} + (\tau_\infty - \tau_m)\sqrt{V(x)}}{\tau_\infty^2\tau_m - \tau_m^2\tau_\infty}.$$

The associated second-order differential operator in time is

$$L_2^\pm(x, \partial_t) = \pm\big(\sqrt{V(x)} - i\alpha_{m,\infty}(x)\partial_t - \beta_{m,\infty}(x)\partial_t^2\big). \tag{3}$$

In Fig. 1, we report the symbols $\lambda_p^\pm$, $\ell_1^\pm$ and $\ell_2^\pm$, with $V(x) = \exp(-x^2)$, for $x \in (-8, 8)$, and $\tau \in (0, \tau_\infty = 20)$ (resp. $\tau \in (0, \tau_\infty = 200)$) with $\tau_m = \tau_\infty/2$, in the region $x \approx 0$. We denote by $\phi_0^\pm$ the restriction of $\phi_{0|\Omega_\varepsilon^\pm}$ to
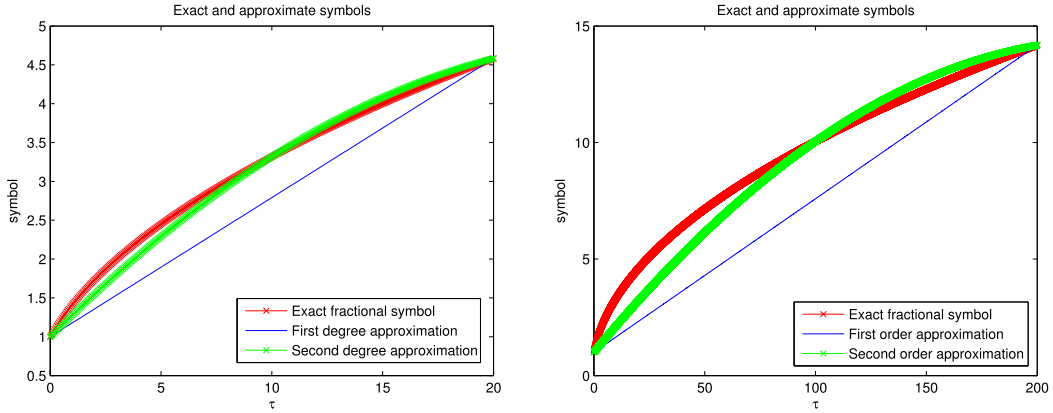
Fig. 1. Principal symbol and Lagrange polynomial approximation of degrees 1 and 2 at $x \approx 0$. Left: $\tau_\infty = 20$. Right: $\tau_\infty = 200$.

$\Omega_\varepsilon^\pm$, with $\Omega_\varepsilon^+ = \left(-\infty, \varepsilon/2\right)$, $\Omega_\varepsilon^- = \left(-\varepsilon/2, +\infty\right)$ and $\varepsilon > 0$ is the size of the overlapping region. For $\kappa = 0$, the OSWR method [5–8] is

$$\begin{cases} P\phi^{\pm,(k)} = 0, & \text{in } \Omega_\varepsilon^\pm \times \mathbb{R}_+^*, \\ \phi^{\pm,(k)}(\cdot, 0) = \phi_0^\pm, & \text{in } \Omega_\varepsilon^\pm, \\ \left(\partial_x + T^\pm(x, \partial_t)\right)\phi^{\pm,(k)}\left(\pm\varepsilon/2, \cdot\right) = \left(\partial_x + T^\pm(x, \partial_t)\right)\phi^{\mp,(k-1)}\left(\pm\varepsilon/2, \cdot\right), & \text{in } \mathbb{R}_+^*, \end{cases}$$

with $T^\pm = \Lambda^\pm$, where the following factorization occurs $P = (\partial_x + \Lambda^-)(\partial_x + \Lambda^+) + \mathcal{R}$, for $P(x, \partial_t) := \mathrm{i}\partial_t + \triangle - V(x)$, and $\mathcal{R} \in \mathrm{OPS}^{-\infty}$ is a smoothing pseudodifferential operator. The SWR algorithm that we propose consists of taking $T^\pm = L_i^\pm$, with $i = 1, 2$, and defined in (2)–(3) which approximate the operator $\Lambda_p^\pm = \mathrm{Op}\left(\lambda_p^\pm\right)$, where $\lambda_p^\pm = \sigma_p(\Lambda^\pm)$. The obvious benefit is that, unlike $\Lambda_p^\pm$, $L_i^\pm$ are local differential operators. Moreover the *Lagrange–Schwarz Waveform Relaxation* (LSWR) method is established without any additional assumption on the time frequency magnitude, unlike OSWR methods. Indeed, although in principle standard OSWR methods [5,8] may be derived independently of the frequency regime, to get explicit expressions of the transmission operators, hypotheses on the frequency are usually necessary. The LSWR method is applied in real-time for the dynamics or in imaginary-time by using the so-called Continuous Normalized Gradient Flow (CNGF) method [2,3,8,12] for computing Hamiltonian operator spectra. The latter needs in addition to the evolution a normalization at each imaginary time step. The Lagrangian polynomials and corresponding differential operators can easily be obtained in imaginary-time [8] by replacing $\tau \to \mathrm{i}\tau$ in $\ell_i^\pm$ and $\partial_t \to \mathrm{i}\partial_t$ in $L_i^\pm$.

We now consider the NLSE (1), with $\kappa > 0$. In [8], we analyzed the convergence rate of the CSWR and OSWR methods in imaginary-time. We show that a polynomial interpolation can still be used for the NLSE to reduce the overall computational complexity of the OSWR methods, but still maintaining a much faster convergence compared to basic CSWR techniques. A natural extension to the transmission operators in the nonlinear case is as follows. The chosen OSWR method is derived by using $\Lambda_p^\pm(x, \partial_t, |\phi|) = \pm\mathrm{Op}\left(\sqrt{\mathrm{i}\partial_t + V + \kappa|\phi|^2}\right)$ [8]. Then a natural extension of the LSWR approach to the NLSE reads for $i = 1, 2$,

$$\begin{cases} P\left(\phi^{\pm,(k)}\right)\phi^{\pm,(k)} = 0, & \text{in } \Omega_\varepsilon^\pm \times \mathbb{R}_+^*, \\ \phi^{\pm,(k)}(\cdot, 0) = \phi_0^\pm, & \text{in } \Omega_\varepsilon^\pm, \\ \left(\partial_x + L_i^\pm\left(x, \partial_t, |\phi^{\pm,(k)}|\right)\right)\phi^{\pm,(k)}\left(\pm\varepsilon/2, \cdot\right) = \left(\partial_x + L_i^\pm\left(x, \partial_t, |\phi^{\mp,(k-1)}|\right)\right)\phi^{\mp,(k-1)}\left(\pm\varepsilon/2, \cdot\right), & \text{in } \mathbb{R}_+^*, \end{cases}$$

where the operators $L_i^\pm$ (which can be used in real or imaginary-time ($t \to \mathrm{i}t$)) are such that

$$L_1^\pm(x, \partial_t, |\phi|) = \pm\left(\sqrt{V + \kappa|\phi|^2} - \mathrm{i}\frac{\sqrt{V + \kappa|\phi|^2 + \tau_\infty} - \sqrt{V + \kappa|\phi|^2}}{\tau_\infty}\partial_t\right),$$

$$L_2^\pm(x, \partial_t, |\phi|)$$

$$= \pm \left(\sqrt{V + \kappa|\phi|^2} - \mathtt{i} \frac{\tau_\infty^2 \sqrt{V + \kappa|\phi|^2 + \tau_m} - \tau_m^2 \sqrt{V + \kappa|\phi|^2 + \tau_\infty} + (\tau_m^2 - \tau_\infty^2)\sqrt{V + \kappa|\phi|^2}}{\tau_\infty^2 \tau_m - \tau_m^2 \tau_\infty} \partial_t \right.$$

$$\left. - \frac{\tau_m \sqrt{V + \kappa|\phi|^2 + \tau_\infty} - \tau_\infty \sqrt{V + \kappa|\phi|^2 + \tau_m} + (\tau_\infty - \tau_m)\sqrt{V + \kappa|\phi|^2}}{\tau_\infty^2 \tau_m - \tau_m^2 \tau_\infty} \partial_t^2 \right). \tag{4}$$

2. Discretization

At the discrete level, we solve (1) on a bounded domain $\Omega_a = (-a, a)$, $a \in \mathbb{R}_+^*$. The subdomains of interest are $\Omega_{a,\varepsilon}^+ = (-a, \varepsilon/2)$, $\Omega_{a,\varepsilon}^- = (-\varepsilon/2, a)$ and $\Omega_a = \Omega_\varepsilon^+ \cup \Omega_\varepsilon^- = (-a, a)$, with the overlapping region $\Gamma_\varepsilon = \Omega_\varepsilon^+ \cap \Omega_\varepsilon^- = (-\varepsilon/2, \varepsilon/2)$, where $\varepsilon \geqslant 0$. The solution ϕ^+ (resp. ϕ^-) in $\Omega_{a,\varepsilon}^+$ (resp. $\Omega_{a,\varepsilon}^-$) at time t_{n+1} and Schwarz iteration k (the time is also denoted by $t_n^{(k)}$ for given (n, k), when necessary) is denoted $\phi^{+,n+1,(k)}$ (resp. $\phi^{-,n+1,(k)}$). The index $\pm\varepsilon/2$ designates a function value at $x = \pm\varepsilon/2$ (such as $\phi_{\pm\varepsilon/2}(\cdot) = \phi(\cdot, \pm\varepsilon/2)$ or $V_{\pm\varepsilon/2} = V(\pm\varepsilon/2)$). As in [8], a Semi-Implicit Euler (SIE) scheme which is unconditionally stable and convergent [2,3,12] is proposed to approximate (1). We denote by Δx (resp. Δt) the space (resp. time) step. For $i = 2$, $L_i^\pm$ requires the approximation of a second-order local time derivative operator. The associated storage at the boundary only needs the approximate solution at t_n and t_{n-1}.

2.1. Lagrange-SWR algorithm

In real-time, the semi-discrete LSWR method writes down

$$\begin{cases} \left(\mathtt{i}\dfrac{I}{\Delta t} + \partial_x^2 - V(x) - \kappa|\phi^{\pm,n,(k)}|^2 \right) \widetilde{\phi}^{\pm,n+1,(k)} = \mathtt{i}\dfrac{\phi^{\pm,n,(k)}}{\Delta t}, \quad \text{in } \Omega_{a,\varepsilon}^\pm, \\ (\partial_x + L_{i,\Delta t}^\pm(x))\left\{ \phi_{\pm\varepsilon/2}^{\pm,n-r+1,(k)} \right\}_{\{0 \leqslant r \leqslant i\}} = (\partial_x + L_{i,\Delta t}^\pm(x))\left\{ \phi_{\pm\varepsilon/2}^{\mp,n-r+1,(k)} \right\}_{\{0 \leqslant r \leqslant i\}}, \\ \phi^{\pm,n+1,(k)} = 0, \quad \text{at } x = \mp a, \end{cases} \tag{5}$$

where the operator $L_{i,\Delta t}^\pm$ is obtained by semi-discretization in time of $L_i^\pm$. The convergence criterion for the Schwarz DDM is set to

$$\left\| \left| \phi_{|\Gamma_\varepsilon}^{+,\text{cvg},(k)} - \phi_{|\Gamma_\varepsilon}^{-,\text{cvg},(k)} \right\|_{\infty,\Gamma_\varepsilon} \right\|_{L^2(0,T)} \leqslant \delta^{\text{Sc}}, \tag{6}$$

with $\delta^{\text{Sc}} = 10^{-14}$ ("Sc" for Schwarz). In imaginary-time, Δt is replaced by $\mathtt{i}\Delta t$ in (5). We then consider a normalized initial guess ϕ_0 and we set $(\widetilde{\phi}^{+,0,(k)}, \widetilde{\phi}^{-,0,(k)}) := (\phi_0^+, \phi_0^-) := (\phi_{0|\Omega_{a,\varepsilon}^+}, \phi_{0|\Omega_{a,\varepsilon}^-})$, for any $k \geqslant 0$. The semi-discrete LSWR-SIE method for a two-domain decomposition of the CNGF is then

$$\begin{cases} \left(\dfrac{I}{\Delta t} - \partial_x^2 + V(x) + \kappa|\phi^{\pm,n,(k)}|^2 \right) \widetilde{\phi}^{\pm,n+1,(k)} = \dfrac{\phi^{\pm,n,(k)}}{\Delta t}, \quad \text{in } \Omega_{a,\varepsilon}^\pm, \\ (\partial_x + L_{i,\Delta t}^\pm(x))\left\{ \widetilde{\phi}_{\pm\varepsilon/2}^{\pm,n-r+1,(k)} \right\}_{\{0 \leqslant r \leqslant i\}} = (\partial_x + L_{i,\Delta t}^\pm(x))\left\{ \widetilde{\phi}_{\pm\varepsilon/2}^{\mp,n-r+1,(k)} \right\}_{\{0 \leqslant r \leqslant i\}}, \\ \widetilde{\phi}^{\pm,n+1,(k)} = 0, \quad \text{at } x = \mp a. \end{cases} \tag{7}$$

At each iteration $(n + 1, k)$, the global solution $\widetilde{\phi}^{n+1,(k)}$ needs to be normalized

$$\phi^{n+1,(k)} := \frac{\widetilde{\phi}^{+,n+1,(k)} + \widetilde{\phi}^{-,n+1,(k)}}{\|\widetilde{\phi}^{+,n+1,(k)} + \widetilde{\phi}^{-,n+1,(k)}\|_{L^2((-a,a))}}. \tag{8}$$

For the CNGF convergence criterion for a given Schwarz iteration k of any SWR-DDM, we stop the computation when $\|\phi^{n+1,(k)} - \phi^{n,(k)}\|_\infty \leqslant \delta$, with δ small enough and $\|\psi\|_\infty := \sup_{x \in \Omega_a} |\psi(x)|$. When

the convergence is reached [8], the stopping time is: $T^{(k)} := T^{\mathrm{cvg},(k)} = n^{\mathrm{cvg},(k)} \Delta t$ for a converged solution $\phi^{\mathrm{cvg},(k)}$ reconstructed from the two subdomains solutions $\phi^{\pm,\mathrm{cvg},(k)}$. In imaginary-time, the convergence criterion for the Schwarz DDM is set to

$$\left\| \left\| \phi_{|\Gamma_\varepsilon}^{+,\mathrm{cvg},(k)} - \phi_{|\Gamma_\varepsilon}^{-,\mathrm{cvg},(k)} \right\|_{\infty,\Gamma_\varepsilon} \right\|_{L^2(0,T^{(k^{\mathrm{cvg}})})} \leqslant \delta^{\mathrm{Sc}}. \tag{9}$$

At the discrete level and in real-time (resp. imaginary-time), we have $\tau_\infty(\Delta t) \approx 1/\Delta t$ (resp. $\tau_\infty(\Delta t) \approx -\mathtt{i}/\Delta t$) and $\tau_m(\Delta t) = 2/\Delta t$ (resp. $\tau_m(\Delta t) = -2\mathtt{i}/\Delta t$). Typically, transmission conditions, for $i = 2$,

$$\left(\partial_x + L_{2,\Delta t}^\pm(x)\right)\left\{\widetilde{\phi}_{\pm\varepsilon/2}^{\pm,n-r+1,(k)}\right\}_{\{0\leqslant r\leqslant 2\}} = \left(\partial_x + L_{2,\Delta t}^\pm(x)\right)\left\{\widetilde{\phi}_{\pm\varepsilon/2}^{\mp,n-r+1,(k)}\right\}_{\{0\leqslant r\leqslant 2\}}$$

are semi-discretized in time at $\pm\varepsilon/2$ as follows

$$\partial_x\phi_{\pm\varepsilon/2}^{\pm,n+1,(k+1)} \pm \sqrt{V_{\pm\varepsilon/2}}\phi_{\pm\varepsilon/2}^{\pm,n+1,(k+1)} - \mathtt{i}\alpha_{m,\infty}(\pm\varepsilon/2,\Delta t)\frac{\phi_{\pm\varepsilon/2}^{\pm,n+1,(k+1)} - \phi_{\pm\varepsilon/2}^{\pm,n,(k+1)}}{\Delta t}$$

$$- \beta_{m,\infty}(\pm\varepsilon/2,\Delta t)\frac{\phi_{\pm\varepsilon/2}^{\pm,n+1,(k+1)} - 2\phi_{\pm\varepsilon/2}^{\pm,n,(k+1)} + \phi_{\pm\varepsilon/2}^{\pm,n-1,(k+1)}}{\Delta t^2}$$

$$= \partial_x\phi_{\pm\varepsilon/2}^{\mp,n+1,(k+1)} \pm \sqrt{V_{\pm\varepsilon/2}}\phi_{\pm\varepsilon/2}^{\mp,n+1,(k+1)} - \mathtt{i}\alpha_{m,\infty}(\pm\varepsilon/2,\Delta t)\frac{\phi_{\pm\varepsilon/2}^{\mp,n+1,(k+1)} - \phi_{\pm\varepsilon/2}^{\mp,n,(k+1)}}{\Delta t}$$

$$- \beta_{m,\infty}(\pm\varepsilon/2,\Delta t)\frac{\phi_{\pm\varepsilon/2}^{\mp,n+1,(k+1)} - 2\phi_{\pm\varepsilon/2}^{\mp,n,(k+1)} + \phi_{\pm\varepsilon/2}^{\mp,n-1,(k+1)}}{\Delta t^2},$$

where

$$\alpha_{m,\infty}(\pm\varepsilon/2,\Delta t) = \frac{\tau_\infty^2(\Delta t)\sqrt{V_{\pm\varepsilon/2} + \tau_m(\Delta t)} - \tau_m^2(\Delta t)\sqrt{V_{\pm\varepsilon/2} + \tau_\infty(\Delta t)} + \left(\tau_m^2(\Delta t) - \tau_\infty^2(\Delta t)\right)\sqrt{V_{\pm\varepsilon/2}}}{\tau_\infty^2(\Delta t)\tau_m(\Delta t) - \tau_m^2(\Delta t)\tau_\infty(\Delta t)}$$

$$\beta_{m,\infty}(\pm\varepsilon/2,\Delta t) = \frac{\tau_m(\Delta t)\sqrt{V_{\pm\varepsilon/2} + \tau_\infty(\Delta t)} - \tau_\infty(\Delta t)\sqrt{V_{\pm\varepsilon/2} + \tau_m(\Delta t)} + \left(\tau_\infty(\Delta t) - \tau_m(\Delta t)\right)\sqrt{V_{\pm\varepsilon/2}}}{\tau_\infty^2(\Delta t)\tau_m(\Delta t) - \tau_m^2(\Delta t)\tau_\infty(\Delta t)}.$$

A Finite Difference Method (FDM) is used in space.

2.2. Optimized SWR algorithm

We summarize here some elements for the discretization of the OSWR method [8]. The transparent operator $\Lambda^\pm$ is approximated by a Taylor expansion assuming $|\tau| \gg 1$ and approximated numerically as follows [8]: $\partial_x\phi + \widetilde{\Lambda}^{+,\ell}(x,t,\partial_x,\partial_t)\phi = 0$, with $\widetilde{\Lambda}^{+,\ell} = \mathrm{Op}(\widetilde{\lambda}^{+,\ell})$, where for the LSE an equivalent form of the ABCs can be obtained (see [13], Corollary 2, page 321) as follows

$$\widetilde{\Lambda}^{+,1}(x,t,\partial_x,\partial_t)\phi = -\mathtt{i}e^{\mathtt{i}\Phi}\partial_t^{1/2}\left(e^{-\mathtt{i}\Phi}\phi\right), \qquad \widetilde{\Lambda}^{+,4}(x,t,\partial_x,\partial_t)\phi = \widetilde{\Lambda}^{+,1}\phi - \frac{\mathtt{i}}{4}\partial_x\left(V(x)\right)e^{\mathtt{i}\Phi}I_t\left(e^{-\mathtt{i}\Phi}\phi\right), \tag{10}$$

where we keep the same notations. The formal extension to the nonlinear case can be found again in [8]. The discretization of the nonlocal time operators is chosen as follows

$$\partial_t^{1/2}f(t_n) \approx \sqrt{\frac{2}{\Delta t}}\sum_{k=0}^n \beta_{n-k}f^k, \qquad I_t f(t_n) \approx \Delta t\sum_{k=1}^n f^k, \tag{11}$$

where the sequence $(\beta_n)_{n\in\mathbb{N}}$ is such that, $\beta_0 = 1$, and for $n \geqslant 0$, $\beta_{n+1} = (-1)^n(1 - 2n)\beta_n/(2n + 2)$. In real-time, the OSWR-SIE method reads

$$\begin{cases} \left(\mathtt{i}\dfrac{I}{\Delta t} + \partial_x^2 - V(x) - \kappa|\phi^{\pm,n,(k)}|^2\right)\widetilde{\phi}^{\pm,n+1,(k)} = \mathtt{i}\dfrac{\phi^{\pm,n,(k)}}{\Delta t}, & \text{in } \Omega_{a,\varepsilon}^\pm, \\[2mm] \left(\pm\partial_x + e^{-\mathtt{i}\pi/4}\sqrt{\dfrac{2}{\Delta t}}\right)\phi_{\pm\varepsilon/2}^{\pm,n+1,(k)} = g_{\pm\varepsilon/2}^{\mp,n+1,(k-1)} + \alpha_{\pm\varepsilon/2}^{\pm,n,(k)} - \alpha_{\pm\varepsilon/2}^{\mp,n,(k-1)}, \\[2mm] \phi^{\pm,n+1,(k)} = 0, & \text{at } x = \mp a, \end{cases} \tag{12}$$
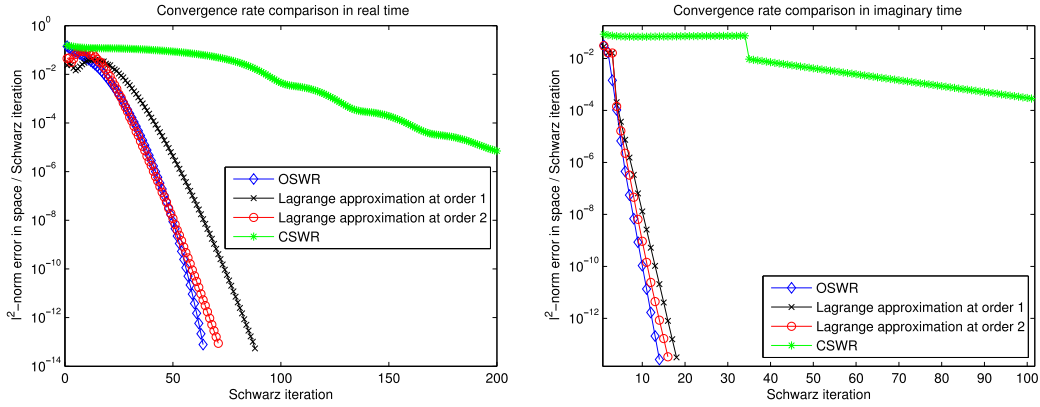
Fig. 2. LSE: comparison of the convergence rates (with $\kappa = 0$) in real-time (left) and imaginary-time (right): OSWR, CSWR and transmission operators with first- and second-order Lagrange polynomials.

where

$$
\begin{aligned}
g_{\pm\varepsilon/2}^{\mp,n+1,(k-1)} &= \pm\partial_x\phi_{\pm\varepsilon/2}^{\mp,n+1,(k-1)} + e^{-\mathrm{i}\pi/4}\sqrt{\frac{2}{\Delta t}}\phi_{\pm\varepsilon/2}^{\mp,n+1,(k-1)}, \\
\alpha_{\pm\varepsilon/2}^{\mp,n,(k)} &= e^{-\mathrm{i}\pi/4} - \sqrt{\frac{2}{\Delta t}}E_{\pm\varepsilon/2}^{\mp,n,(k)}\sum_{\ell=0}^{n}\beta_{n+1-\ell}\bar{E}_{\pm\varepsilon/2}^{\mp,\ell,(k)}\phi_{\pm\varepsilon/2}^{\mp,\ell,(k)}, \\
E_{\pm\varepsilon/2}^{\mp,n,(k)} &= \exp\left(-\Delta t\sum_{q=0}^{n}(V_{\pm\varepsilon/2}+\kappa|\phi_{\pm\varepsilon/2}^{\mp,q,(k)}|^2)\right), \qquad \bar{E}_{\pm\varepsilon/2}^{\mp,n,(k)} = \frac{1}{E_{\pm\varepsilon/2}^{\mp,n,(k)}}.
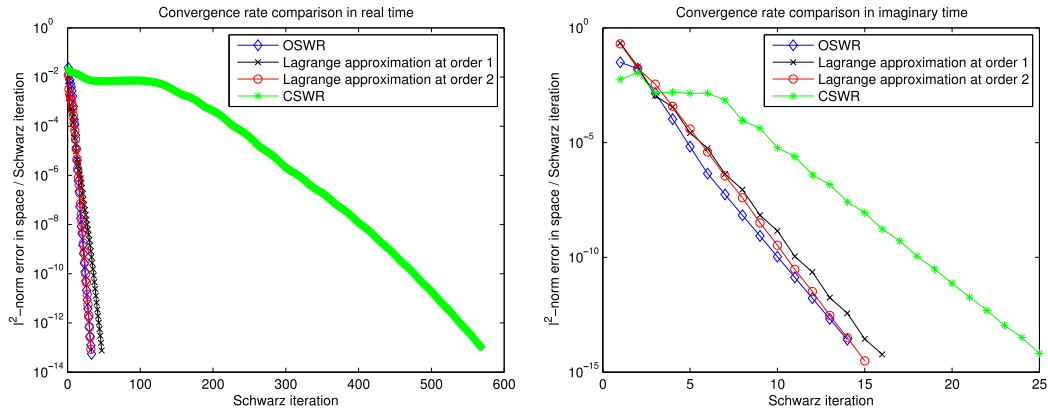\end{aligned}
\tag{13}
$$

Let us remark that the computational complexity for updating the transmission conditions is *proportional to the number of time iterations* and needs the *storage of the solution at the interface at all time*. As it is well-known, this naturally constitutes a fundamental computational complexity issue in higher dimension and leads to possible stability problems. In imaginary-time, we refer to [8] for a full description of the OSWR-SIE scheme for LSE/NLSE.

3. Numerical experiments

We solve (1) on $(-8, 8)$ in imaginary-time for computing the ground state of the Hamiltonian operator and in real-time for a wavepacket evolution. Homogeneous Dirichlet boundary conditions are imposed at ± 8. For the LSE, we consider $V(x) = x^2/2 + 25\sin^2(\pi x/2)$ and $\kappa = 0$ (resp. NLSE $V(x) = x^2$ and $\kappa = 100$). The initial data is given by $\exp(-x^2)\pi^{-1/4}$. A semi-implicit Euler scheme approximates (1), with $\Delta t = 0.1$ and $\Delta x = 16/255$. In real-time, the final time is $T = 5$. The size of the overlapping region is fixed to $\varepsilon = \Delta x$. At the subdomain interfaces, we impose the transmission operator $\partial_x + T^{\pm}(x, \partial_t)$, with $T^{\pm}(x, \partial_t) = \widetilde{\Lambda}^{\pm,4}(x, \partial_t)$ (OSWR) see (10), $T^{\pm}(x, \partial_t) = L_i^{\pm}(x, \partial_t)$ ($i = 1, 2$, LSWR) and $T^{\pm}(x, \partial_t) = \pm\mathrm{I}$ (CSWR). Notice that to start the time iteration in the case $i = 2$, as ϕ_0 is the unique available Cauchy data, we use L_1 rather than L_2.

We first consider that $\kappa = 0$. In Fig. 2-left (resp. Fig. 2-right), we compare the convergence rates of the OSWR, CSWR and LSWR methods with respect to the Schwarz iteration k, i.e. (6) in real-time and (9) in imaginary-time. We remark that as expected OSWR provides the fastest convergence rate but the approximation of the exact principal symbol $\lambda_p^{\pm}$ by low order Lagrange polynomials also leads to a fast convergence. In both cases, the more accurate the Lagrange interpolation, the faster the convergence.

Next, we consider $\kappa = 100$ in real-(resp. imaginary-)time and compare in Fig. 3-left (resp. Fig. 3-right) the rates of convergence of the OSWR, LSWR and CSWR methods for the transmission operators, with respectively $T^{\pm}(x, \partial_t, |\phi|) = \widetilde{\Lambda}^{\pm,4}(x, \partial_t, |\phi|)$, $T^{\pm}(x, \partial_t, |\phi|) = L_i^{\pm}(x, \partial_t, |\phi|)$ ($i = 1, 2$) and $T^{\pm}(x, \partial_t, |\phi|) = \pm\mathrm{I}$.

Fig. 3. NLSE: comparison of the convergence rates (with $\kappa = 100$) in real-time (left) and imaginary-time (right): OSWR, CSWR and transmission operators with first- and second-order Lagrange polynomials.

As in the linear case, we observe that the LSWR approach provides almost the same convergence rate as for the OSWR method. Let us notice that the overall convergence rate is very fast in imaginary-time, even for the CSWR which is due to the large value of κ (see [8] for further explanations).

4. Conclusion

In this letter, we have shown that approximating symbols of transparent transmission operators by low-order Lagrange interpolation polynomials leads to the construction of efficient discrete Schwarz waveform relaxation domain decomposition methods. Using low order Lagrange polynomials, LSWR methods almost exhibit the same convergence rates as for the OSWR techniques for the LSE/NLSE. This promising methodology will be analyzed and tested on larger scales and higher dimensional problems.

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