A fast solution method for time dependent multi-dimensional Schroedinger equations

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Abstract. In this paper we propose fast solution methods for the Cauchy problem for the multi-dimensional Schrödinger equation. Our approach is based on the approximation of the data by the basis functions introduced in the theory of approximate approximations. We obtain high order approximations also in higher dimensions up to a small saturation error, which is negligible in computations, and we prove error estimates in mixed Lebesgue spaces for the inhomogeneous equation. The proposed method is very efficient in high dimensions if the densities allow separated representations. We illustrate the efficiency of the procedure on different examples, up to approximation order 6 and space dimension 200.

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1 Introduction

The evolution of the wave function $u(\mathbf{x},t)$ of a free particle in quantum mechanics is described by the Schrödinger equation

$$i\frac{\partial u}{\partial t} + \Delta_{\mathbf{x}} u = 0\,. \tag{1.1}$$

Equation (1.1) has also important applications in optics, underwater acoustics, electromagnetic wave propagation (cf. e.g. [1] and the reference therein).

In this paper we propose fast solution methods for the Cauchy problem of (1.1)

$$u(\mathbf{x},0) = g(\mathbf{x}), \quad \mathbf{x} = (x_1,,\ldots,x_n) \in \mathbb{R}^n, \tag{1.2}$$

and for the inhomogeneous Schrödinger equation

$$i\frac{\partial u}{\partial t} + \Delta_{\mathbf{x}} u = f(\mathbf{x},t), \quad (\mathbf{x},t) \in \mathbb{R}^n \times \mathbb{R}_+ \,. \tag{1.3}$$

Under suitable integrability or decay conditions on g and f the solution of (1.1) - (1.2) can be written as

$$u(\mathbf{x},t) = \mathcal{S}g(\mathbf{x},t) = \int\limits_{\mathbb{R}^n} \mathcal{K}(\mathbf{x}-\mathbf{y},t)\, g(\mathbf{y})\, d\mathbf{y}\,, \tag{1.4}$$

and the solution of (1.3) - (1.2) is given by

$$u(\mathbf{x},t) = \mathcal{S}g(\mathbf{x},t) + \Pi f(\mathbf{x},t)$$

with

$$\Pi f(\mathbf{x},t) = -i\int\limits_0^t ds \int\limits_{\mathbb{R}^n} \mathcal{K}(\mathbf{x}-\mathbf{y},t-s) f(\mathbf{y},s)\, d\mathbf{y}\, ds = -i\int\limits_0^t (\mathcal{S}f(\cdot,s))(\mathbf{x},t-s)\, ds\,. \tag{1.5}$$

Here $\mathcal{K}(\mathbf{x},t)$ denotes the fundamental solution of (1.1) [7, p.193]

$$\mathcal{K}(\mathbf{x},t) = \frac{\mathrm{e}^{\,i\,|\mathbf{x}|^2/(4t)}}{(4\pi i t)^{n/2}}\,.$$

In terms of the Fourier transform

$$\mathcal{F}u(\boldsymbol{\xi}) = \int\limits_{\mathbb{R}^n} u(\mathbf{x})\, \mathrm{e}^{-2\pi i\langle \mathbf{x},\boldsymbol{\xi}\rangle}\, d\mathbf{x}$$

the integral operators $\mathcal{S}$ and Π can be written as follows:

$$\mathcal{S}g(\mathbf{x},t) = \int\limits_{\mathbb{R}^n} \mathrm{e}^{2\pi i\langle \mathbf{x},\boldsymbol{\xi}\rangle} \mathrm{e}^{-4\pi^2 it|\boldsymbol{\xi}|^2} \mathcal{F}g(\boldsymbol{\xi})\, d\boldsymbol{\xi}\,, \tag{1.6}$$

$$\Pi f(\mathbf{x},t) = -i\int\limits_0^t ds \int\limits_{\mathbb{R}^n} \mathrm{e}^{2\pi i\langle \mathbf{x},\boldsymbol{\xi}\rangle} \mathrm{e}^{-4\pi^2 i\,(t-s)|\boldsymbol{\xi}|^2} \mathcal{F}f(\boldsymbol{\xi},s)\, d\boldsymbol{\xi}\,.$$

For fixed $t > 0$ the integral operator $\mathcal{S}$ is bounded in $L^p = L^p(\mathbb{R}^n)$ spaces. From (1.4) and (1.6) it follows immediately that

$$\|\mathcal{S}g(\cdot,t)\|_{L^\infty} \le \frac{1}{(4\pi|t|)^{n/2}} \|g\|_{L^1}\,, \quad \|\mathcal{S}g(\cdot,t)\|_{L^2} = \|g\|_{L^2}\,,$$

hence by interpolation the L^p dispersive estimate

$$\|\mathcal{S}g(\cdot,t)\|_{L^p} \le C|t|^{-n(1/2-1/p)} \|g\|_{L^{p'}}\,, \quad t \ne 0\,, \tag{1.7}$$

holds for $2 \le p \le \infty$ and p' is the adjoint exponent, $1/p + 1/p' = 1$.

Estimates of norms of solutions $u(\mathbf{x},t)$ on $\mathbb{R}^n \times \mathbb{R}$ are known for example in mixed Lebesgue spaces. For an interval I and $r, q \geq 1$, $L^{r,q}(I)$ denotes the Banach space of $L^r(\mathbb{R}^n)$-valued q-summable functions over I with the norm

$$\|u\|_{L^{r,q}(I)} = \|u\|_{r,q} = \Big(\int\limits_I \Big(\int\limits_{\mathbb{R}^n} |u(\mathbf{x},t)|^r d\mathbf{x} \Big)^{q/r} dt \Big)^{1/q} .$$

The exponent pair (q,r) is called Schrödinger-admissible if $q, r \geq 2$, $(q,r) \neq (2,\infty)$ and

$$\frac{2}{q} + \frac{n}{r} = \frac{n}{2} . \tag{1.8}$$

For any Schrödinger-admissible pairs (q,r) Strichartz type estimates

$$\|\mathcal{S}g\|_{L^{r,q}(\mathbb{R}_+)} \leq C\|g\|_{L^2} , \quad \|\Pi f\|_{L^{r,q}(\mathbb{R}_+)} \leq C\|f\|_{L^{r',q'}(\mathbb{R}_+)} \tag{1.9}$$

are valid with constants C independent of $g \in L^2(\mathbb{R}^n)$ and $f \in L^{r',q'}(\mathbb{R}_+)$, [8, (11)]. Moreover, $u = \mathcal{S}g + \Pi f$ is continuous in t in the space L^2 and

$$\sup_{t\in\mathbb{R}_+} \|u(\cdot,t)\|_{L^2} \leq C(\|g\|_{L^2} + \|f\|_{L^{r',q'}(\mathbb{R}_+)}) .$$

Note that for $q = r = 2 + 4/n$ we derive the classical Strichartz estimate [16]

$$\|u\|_{L^{2(n+2)/n}} = \Big(\int\limits_{\mathbb{R}_+} \int\limits_{\mathbb{R}^n} |u(\mathbf{x},t)|^{2(n+2)/n} d\mathbf{x} dt \Big)^{n/(2(n+2))} \leq C\big(\|g\|_{L_2} + \|f\|_{L^{2(n+2)/(n+4)}}\big) .$$

The goal of this paper is to derive semi-analytic cubature formulas for $\mathcal{S}g$ in (1.4) and Πf in (1.5) of an arbitrary high order which are fast and accurate also if the space dimension $n \geq 3$. We follow the philosophy introduced in [9] and [10] for the cubature of high-dimensional Newton potential over the full space and over half-spaces. The idea is to approximate the density functions by the basis functions introduced in the theory of *approximate approximations* (cf. [14] and the references therein). This approach, combined with *separated representations* (cf. [4] and [5]) makes the method fast and successful in high dimensions. In [11] and [12] we applied this procedure to obtain cubature formulas for advection-diffusion operators over rectangular boxes in $\mathbb{R}^n$. In [13] our approach was extended to parabolic problems. For the Schrödinger equation the situation is different because the fundamental solution does not decay exponentially and standard cubature methods are very expansive due to the oscillations of the kernel, especially in multi-dimensional case. The application of approximate approximations to this equation reduces these problems and provides new very efficient semi-analytic cubature formulas.

The article is organized as follows. In section 2, after an introduction into simple cubature formulas for the operators $\mathcal{S}$ and Π based on *approximate quasi-interpolants*, we prove estimates of the cubature error for general generating functions. Similar to other integral operators of potential theory, we obtain high order approximations also in higher dimensions up to a small saturation error, which is negligible in computations. In section 3 we describe algorithms for high-order approximations of (1.4) and (1.5). Using the tensor product structure of cubature formulas, these algorithms are very efficient in high dimensions, if g and f allow separate representations. The approach is extended in section 4 to the case that g and f are supported with respect to $\mathbf{x}$ in a hyper-rectangle on $\mathbb{R}^n$. In Section 5 we illustrate the efficiency of the method on several examples, up to approximation order 6 and space dimension 200. For the two-dimensional initial value problem (1.1) we provide graphics of the evolution of $u(\mathbf{x},t)$.

2 Cubature of $\mathcal{S}g$ and Πf

2.1 Approximate quasi-interpolants

To find an approximate solution of (1.1) - (1.2) we replace the function g in (1.4) by an approximate quasi-interpolant

$$(\mathcal{M}_{h\sqrt{\mathcal{D}}}\, g)(\mathbf{x}) = \mathcal{D}^{-n/2} \sum_{\mathbf{m}\in\mathbb{Z}^n} g(h\mathbf{m})\eta\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\Big), \tag{2.1}$$

where η is a rapidly decaying function of the Schwarz space $S(\mathbb{R}^n)$ satisfying for positive integer N the moment condition

$$\int\limits_{\mathbb{R}^n} \eta(\mathbf{x})\, d\mathbf{x} = 1\,, \int\limits_{\mathbb{R}^n} \mathbf{x}^{\boldsymbol{\alpha}}\eta(\mathbf{x})\, d\mathbf{x} = 0, \quad \forall\, \boldsymbol{\alpha}\,,\ 1 \le |\boldsymbol{\alpha}| < N\,. \tag{2.2}$$

Here and in the following we use multi-index notation, bold Greek letters denote multi-indices. Then the function

$$\begin{aligned} \mathcal{S}_h g(\mathbf{x},t) &= \mathcal{S}(\mathcal{M}_{h\sqrt{\mathcal{D}}}\, g)(\mathbf{x},t) \\ &= \frac{1}{\mathcal{D}^{n/2}(4\pi i t)^{n/2}} \sum_{\mathbf{m}\in\mathbb{Z}^n} g(h\mathbf{m}) \int\limits_{\mathbb{R}^n} \mathrm{e}^{i\,|\mathbf{x}-\mathbf{y}|^2/(4t)}\eta\Big(\frac{\mathbf{y}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\Big)d\mathbf{y} \end{aligned} \tag{2.3}$$

can be considered as cubature of $\mathcal{S}g$, if η is chosen such that $\mathcal{S}\eta(\mathbf{x},t)$ can be computed easily, preferably as an analytic expression. The existence of those generating functions η has been shown for various integral operators.

Then the cubature error follows immediately from the quasi-interpolation error due to

$$\mathcal{S}g(\cdot,t) - \mathcal{S}_h g(\cdot,t) = \mathcal{S}(I - \mathcal{M}_{h\sqrt{\mathcal{D}}})\, g(\cdot,t)\,.$$

Approximation properties of quasi-interpolants of the form (2.1) have been studied in the framework of approximate approximations (cf. [14]). Let us recall the structure of the quasi-interpolation error, which is proved in general form in [14, Thm 2.28]. Suppose that g has generalized derivatives of order N. Using Taylor expansions of $g(\mathbf{x})$ for the nodes $h\mathbf{m}$, $\mathbf{m}\in\mathbb{Z}^n$, and Poisson's summation formula the quasi-interpolant can be written as

$$(\mathcal{M}_{h\sqrt{\mathcal{D}}}\, g)(\mathbf{x}) = (-h\sqrt{\mathcal{D}})^N g_N(\mathbf{x}) + \sum_{|\boldsymbol{\alpha}|=0}^{N-1} \frac{(h\sqrt{\mathcal{D}})^{|\boldsymbol{\alpha}|}}{\boldsymbol{\alpha}!(2\pi i)^{|\boldsymbol{\alpha}|}}\, \partial^{\boldsymbol{\alpha}} g(\mathbf{x})\, \sigma_{\boldsymbol{\alpha}}(\mathbf{x},\eta,\mathcal{D}) \tag{2.4}$$

with the function

$$g_N(\mathbf{x}) = \frac{1}{\mathcal{D}^{n/2}} \sum_{|\boldsymbol{\alpha}|=N} \frac{N}{\boldsymbol{\alpha}!} \sum_{\mathbf{m}\in\mathbb{Z}^n} \Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\Big)^{\boldsymbol{\alpha}} \eta\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\Big) \int\limits_0^1 s^{N-1}\partial^{\boldsymbol{\alpha}} g(s\mathbf{x}+(1-s)h\mathbf{m})\, ds\,,$$

containing the remainder of the Taylor expansions, and the fast oscillating functions

$$\sigma_{\boldsymbol{\alpha}}(\mathbf{x},\eta,\mathcal{D}) = \frac{1}{\mathcal{D}^{n/2}} \sum_{\mathbf{m}\in\mathbb{Z}^n} \Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\Big)^{\boldsymbol{\alpha}} \eta\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\Big) = \sum_{\boldsymbol{\nu}\in\mathbb{Z}^n} \partial^{\boldsymbol{\alpha}}\mathcal{F}\eta(\sqrt{\mathcal{D}}\boldsymbol{\nu})\, \mathrm{e}^{\frac{2\pi i}{h}\langle \mathbf{x},\boldsymbol{\nu}\rangle}\,. \tag{2.5}$$

If $g \in W_p^N(\mathbb{R}^n)$ with $N > n/p$, $1 \le p \le \infty$, then g_N can be estimated by

$$\|g_N\|_{L_p} \le C_N \sum_{|\boldsymbol{\alpha}|=N} \|\partial^{\boldsymbol{\alpha}} g\|_{L_p} = C_N |g|_{W_p^N}$$

with a constant C_N depending only on η, n, and p. It follows from (2.5) that due to the moment condition (2.2) the second sum in (2.4) transforms to

$$g(\mathbf{x}) + \sum_{|\boldsymbol{\alpha}|=0}^{N-1} \frac{(h\sqrt{\mathcal{D}})^{|\boldsymbol{\alpha}|}}{\boldsymbol{\alpha}!(2\pi i)^{|\boldsymbol{\alpha}|}} \, \partial^{\boldsymbol{\alpha}} g(\mathbf{x}) \, \epsilon_{\boldsymbol{\alpha}}(\mathbf{x}, \eta, \mathcal{D}) \,,$$

where we denote

$$\epsilon_{\boldsymbol{\alpha}}(\mathbf{x}, \eta, \mathcal{D}) = \sum_{\substack{\boldsymbol{\nu} \in \mathbb{Z}^n \\ \boldsymbol{\nu} \ne 0}} \partial^{\boldsymbol{\alpha}} \mathcal{F}\eta(\sqrt{\mathcal{D}}\boldsymbol{\nu}) \, \mathrm{e}^{\frac{2\pi i}{h}\langle \mathbf{x}, \boldsymbol{\nu}\rangle} = \sigma_{\boldsymbol{\alpha}}(\mathbf{x}, \eta, \mathcal{D}) - \delta_{0|\boldsymbol{\alpha}|} \,.$$

Hence (2.4) leads to the representation of the quasi-interpolation error

$$(\mathcal{M}_{h\sqrt{\mathcal{D}}}\, g)(\mathbf{x}) - g(\mathbf{x}) = (-h\sqrt{\mathcal{D}})^N g_N(\mathbf{x}) + \sum_{|\boldsymbol{\alpha}|=0}^{N-1} \frac{(h\sqrt{\mathcal{D}})^{|\boldsymbol{\alpha}|}}{\boldsymbol{\alpha}!(2\pi i)^{|\boldsymbol{\alpha}|}} \, \partial^{\boldsymbol{\alpha}} g(\mathbf{x}) \epsilon_{\boldsymbol{\alpha}}(\mathbf{x}, \mathcal{D}, \eta),$$

which implies in particular the error estimate in $L^p(\mathbb{R}^n)$

$$\|g - \mathcal{M}_{h\sqrt{\mathcal{D}}}\, g\|_{L^p} \le C_N (h\sqrt{\mathcal{D}})^N |g|_{W_p^N} + \sum_{k=0}^{N-1} \frac{(h\sqrt{\mathcal{D}})^k}{(2\pi)^k} \sum_{|\boldsymbol{\alpha}|=k} \frac{\|\epsilon_{\boldsymbol{\alpha}}(\cdot, \mathcal{D}, \eta)\|_{L^\infty} \|\partial^{\boldsymbol{\alpha}} g\|_{L^p}}{\boldsymbol{\alpha}!} \,. \tag{2.6}$$

Thus the quasi-interpolation error consists of a term ensuring $\mathcal{O}(h^N)$-convergence and of the so-called saturation error, which, in general, does not converge to zero as $h \to 0$. However, due to the fast decay of $\partial^{\boldsymbol{\alpha}} \mathcal{F}\eta$, one can choose $\mathcal{D}$ large enough to ensure that

$$\|\epsilon_{\boldsymbol{\alpha}}(\cdot, \mathcal{D}, \eta)\|_{L^\infty} \le \sum_{\boldsymbol{\nu} \in \mathbb{Z}^n \setminus \mathbf{0}} |\partial^{\boldsymbol{\alpha}} \mathcal{F}\eta(\sqrt{\mathcal{D}}\boldsymbol{\nu})| < \varepsilon$$

for given small $\varepsilon > 0$. In the examples below the saturation error is of the order $\mathcal{O}(\mathrm{e}^{-\pi^2 \mathcal{D}})$, which in the cases $\mathcal{D} = 2$ and $\mathcal{D} = 4$ is comparable to the single and double precision arithmetics of modern computers. Therefore, in numerical computations the saturation error can be neglected for appropriately chosen $\mathcal{D}$.

2.2 Approximation error for $\mathcal{S}g$

From (2.3) we see that

$$\mathcal{S}_h g(\mathbf{x}, t) = \mathcal{D}^{-n/2} \sum_{\mathbf{m} \in \mathbb{Z}^n} g(h\mathbf{m}) \, \mathcal{S}\eta\Big(\frac{\mathbf{x} - h\mathbf{m}}{h\sqrt{\mathcal{D}}}, \frac{t}{h^2 \mathcal{D}}\Big). \tag{2.7}$$

Hence, if $\mathcal{S}\eta(\mathbf{x}, t)$ is known analytically, then (2.7) is a very simple semi-analytic cubature of $\mathcal{S}g$. Of course, the cubature formula is computable only for a finite number of nonvanishing terms in (2.7). Therefore we assume that $g(\mathbf{x})$ and $f(\mathbf{x}, t)$ are compactly supported.

The mapping properties (1.7) and (1.9) of $\mathcal{S}$ and the quasi-interpolation error (2.6) lead to estimates of the approximation error for $\mathcal{S}g$. In the following theorem we use the notation

$$\|\nabla_k g\|_{L^p} = \sum_{|\boldsymbol{\alpha}|=k} \frac{\|\partial^{\boldsymbol{\alpha}} g\|_{L^p}}{\boldsymbol{\alpha}!}\,.$$

Theorem 2.1. *Let $g \in W_p^N(\mathbb{R}^n)$, $1 \le p \le 2$, $N > n/p$, be the initial value for the homogeneous Schrödinger equation (1.1). For any $\varepsilon > 0$ there exists $\mathcal{D} > 0$ such that for $t > 0$ the cubature formula (2.7) approximates the solution $u(\mathbf{x}, t)$ in $L^{p'}(\mathbb{R}^n)$, $p' = p/(p-1)$, with*

$$\|u(\cdot,t) - \mathcal{S}_h g(\cdot,t)\|_{L^{p'}} \le \frac{C}{t^{n(1/2-1/p')}}\Big((h\sqrt{\mathcal{D}})^N |g|_{W_p^N} + \varepsilon \sum_{k=0}^{N-1} \frac{(h\sqrt{\mathcal{D}})^k}{(2\pi)^k} \|\nabla_k g\|_{L^p}\Big).$$

Moreover, if $g \in W_2^N(\mathbb{R}^n)$, then the approximation on $\mathbb{R}^n \times \mathbb{R}$ with $u_h(\mathbf{x},t) = \mathcal{S}_h g(\mathbf{x},t)$ can be estimated in the mixed Lebesgue spaces $L^{r,q}(\mathbb{R}_+)$ for any Schrödinger-admissible pairs (q,r), cf. (1.8), by

$$\|u - u_h\|_{L^{r,q}(\mathbb{R}_+)} \le C\Big((h\sqrt{\mathcal{D}})^N |g|_{W_2^N} + \varepsilon \sum_{k=0}^{N-1} \frac{(h\sqrt{\mathcal{D}})^k}{(2\pi)^k} \|\nabla_k g\|_{L^2}\Big).$$

Remark 2.1. *The analysis of the application of the integral operator $\mathcal{S}$ on the saturation error*

$$R_N(\mathbf{x}) = \sum_{|\boldsymbol{\alpha}|=0}^{N-1} \frac{(h\sqrt{\mathcal{D}})^{|\boldsymbol{\alpha}|}}{\boldsymbol{\alpha}!(2\pi i)^{|\boldsymbol{\alpha}|}}\, \partial^{\boldsymbol{\alpha}} g(\mathbf{x})\, \epsilon_{\boldsymbol{\alpha}}(\mathbf{x}, \eta, \mathcal{D})$$

shows, that $|\mathcal{S}R_N(\mathbf{x},t)| \to 0$ for fixed $(\mathbf{x},t)$ as $h \to 0$. For example, if $(1+|\mathbf{x}|^2)^{(N-1)/2} g(\mathbf{x}) \in W_1^{N-1}(\mathbb{R}^n)$, then $|\mathcal{S}R_N(\mathbf{x},t)| = Ct^{-n/2}(\sqrt{\mathcal{D}}h)^N \|(1+|\cdot|^2)^{(N-1)/2} g\|_{W_1^{N-1}}$ for all $|\mathbf{x}| < 2\pi t/h$.

2.3 Approximation error for Πf

We construct an approximation for Πf in (1.5) using the approximate quasi-interpolant

$$\mathcal{N}_{h\sqrt{\mathcal{D}},\tau\sqrt{\mathcal{D}_0}} f(\mathbf{x},t) = \frac{1}{\sqrt{\mathcal{D}_0 \mathcal{D}^n}} \sum_{\substack{\ell\in\mathbb{Z}\\ \mathbf{m}\in\mathbb{Z}^n}} f(h\mathbf{m}, \tau\ell)\, \psi\Big(\frac{t-\tau\ell}{\tau\sqrt{\mathcal{D}_0}}\Big)\eta\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\Big). \tag{2.8}$$

Here τ, h, are the step sizes, $\mathcal{D}_0$ and $\mathcal{D}$ are positive fixed parameters; $\psi \in S(\mathbb{R})$ and $\eta \in S(\mathbb{R}^n)$ are the generating functions, which belong to the Schwartz space S of smooth and rapidly decaying functions. If the generating functions ψ and η fulfills the moment condition (2.2) of order N, then $\mathcal{N}_{h\sqrt{\mathcal{D}},\tau\sqrt{\mathcal{D}_0}} f$ approximates f with the order $\mathcal{O}((h\sqrt{\mathcal{D}}+\tau\sqrt{\mathcal{D}_0})^N)$ up to the saturation error in $L^p(\mathbb{R}^{n+1})$ if $N > (n+1)/p$. This is also true for mixed Lebesgue spaces, which are used for the mapping properties (1.9) of Π.

More precisely, using the previously mentioned approach one can expand

$$(\mathcal{N}_{h\sqrt{\mathcal{D}},\tau\sqrt{\mathcal{D}_0}} f)(\mathbf{x},t) = f_N(\mathbf{x},t) + \mathcal{R}_N f(\mathbf{x},t)\,,$$

where

$$f_N(\mathbf{x},t) = \frac{(-1)^N N}{\sqrt{\mathcal{D}_0\mathcal{D}^n}} \sum_{k=0}^{N} \frac{(\tau\sqrt{\mathcal{D}_0})^k (h\sqrt{\mathcal{D}})^{N-k}}{k!}$$
$$\times \sum_{|\boldsymbol{\alpha}|=N-k} \frac{1}{\boldsymbol{\alpha}!} \sum_{\substack{\ell\in\mathbb{Z}\\ \mathbf{m}\in\mathbb{Z}^n}} \Big(\frac{t-\tau\ell}{\tau\sqrt{\mathcal{D}_0}}\Big)^k \psi\Big(\frac{t-\tau\ell}{\tau\sqrt{\mathcal{D}_0}}\Big)\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\Big)^{\boldsymbol{\alpha}} \eta\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\Big) U_{k,\boldsymbol{\alpha}}(\mathbf{x},h\mathbf{m},t,\tau\ell)$$

with the notation

$$U_{k,\boldsymbol{\alpha}}(\mathbf{x},\mathbf{y},t,z) = \int_0^1 s^{N-1} \partial_{\mathbf{x}}^{\boldsymbol{\alpha}} \partial_t^k f\big(s\mathbf{x}+(1-s)\mathbf{y}, st+(1-s)z\big)\, ds\,,$$

and the function

$$\mathcal{R}_N f(\mathbf{x},t) = \sum_{k=0}^{N-1} \frac{(\tau\sqrt{\mathcal{D}_0})^k\, \sigma_k(t,\psi,\mathcal{D}_0)}{k!\,(2\pi i)^k} \sum_{|\boldsymbol{\alpha}|=0}^{N-1-k} \frac{(h\sqrt{\mathcal{D}})^{|\boldsymbol{\alpha}|}\, \sigma_{\boldsymbol{\alpha}}(\mathbf{x},\eta,\mathcal{D})}{\boldsymbol{\alpha}!\,(2\pi i)^{|\boldsymbol{\alpha}|}}\, \partial_{\mathbf{x}}^{\boldsymbol{\alpha}} \partial_t^k f(\mathbf{x},t)\,.$$

The moment conditions for ψ and η obviously imply, that for $q,r\in[1,\infty]$ and f such that the partial derivatives $\partial_{\mathbf{x}}^{\boldsymbol{\alpha}}\partial_t^k f \in L^{r,q}(\mathbb{R})$ for all indices $|\boldsymbol{\alpha}|+k\le N$,

$$\begin{aligned}\|\mathcal{R}_N f - f\|_{L^{r,q}} \le \|\sigma_{\mathbf{0}}(\cdot,\mathcal{D},\eta)\|_{L^\infty} \sum_{k=0}^{N-1} \frac{(\tau\sqrt{\mathcal{D}_0})^k}{k!\,(2\pi)^k}\, \|\epsilon_k(\cdot,\mathcal{D}_0,\psi)\|_{L^\infty} \|\partial_t^k f\|_{L^{r,q}} \\ + \|\sigma_0(\cdot,\mathcal{D}_0,\psi)\|_{L^\infty} \sum_{k=0}^{N-1} \frac{(h\sqrt{\mathcal{D}})^k}{(2\pi)^k} \sum_{|\boldsymbol{\alpha}|=k} \frac{\|\epsilon_{\boldsymbol{\alpha}}(\cdot,\mathcal{D},\eta)\|_{L^\infty}}{\boldsymbol{\alpha}!}\, \|\partial_{\mathbf{x}}^{\boldsymbol{\alpha}} f\|_{L^{r,q}} \\ + \sum_{k=1}^{N-1} \frac{(\tau\sqrt{\mathcal{D}_0})^k \|\epsilon_k(\cdot,\mathcal{D}_0,\psi)\|_{L^\infty}}{k!\,(2\pi)^k} \sum_{|\boldsymbol{\alpha}|=1}^{N-1-k} \frac{(h\sqrt{\mathcal{D}})^{|\boldsymbol{\alpha}|}\|\epsilon_{\boldsymbol{\alpha}}(\cdot,\mathcal{D},\eta)\|_{L^\infty}}{\boldsymbol{\alpha}!(2\pi)^{|\boldsymbol{\alpha}|}} \|\partial_{\mathbf{x}}^{\boldsymbol{\alpha}}\partial_t^k f\|_{L^{r,q}}\,.\end{aligned}$$

Moreover, if $N > (n+1)/\min(q,r)$, then one can show similar to [14, Lemma 2.29] that

$$\|f_N\|_{L^{r,q}} \le C \sum_{k=0}^{N} \sum_{|\boldsymbol{\alpha}|=N-k} (\tau\sqrt{\mathcal{D}_0})^k (h\sqrt{\mathcal{D}})^{N-k} \|\partial_t^k \partial_{\mathbf{x}}^{\boldsymbol{\alpha}} f\|_{L^{r,q}}\,.$$

Now we are in the position to study the approximation of Πf defined by

$$\Pi_{h,\tau} f(\mathbf{x},t) = \Pi(\mathcal{N}_{h\sqrt{\mathcal{D}},\tau\sqrt{\mathcal{D}_0}} f)(\mathbf{x},t) = -i \int_0^t ds \int_{\mathbb{R}^n} \mathcal{K}(\mathbf{x}-\mathbf{y},t-s)\, \mathcal{N}_{h\sqrt{\mathcal{D}},\tau\sqrt{\mathcal{D}_0}} f(\mathbf{y},s)\, d\mathbf{y}\,.$$

Then the difference between Πf and $\Pi_{h,\tau} f$ can be estimated by (1.9) and the quasi-interpolation error $\|f - \mathcal{N}_{h\sqrt{\mathcal{D}},\tau\sqrt{\mathcal{D}_0}} f\|_{L^{r',q'}}$. However, the corresponding error estimate is proved for sufficiently smooth functions on $\mathbb{R}^{n+1}$, whereas the right-hand side f of (1.3) is given only on $\mathbb{R}^n \times \mathbb{R}_+$. Therefore we extend $f(\cdot,t): \mathbb{R}_+ \to W_r^N(\mathbb{R}^n)$ with preserved smoothness to a function $f(\cdot,t): \mathbb{R} \to W_r^N(\mathbb{R}^n)$. This can be done, for example, by using Hestenes reflection principle (cf. [6]

and (5.3)). The extended function, again denoted by f, is compactly supported and retains the smoothness of $f|_{\mathbb{R}^n\times\mathbb{R}_+}$. Then we get

$$\Pi_{h,\tau} f(\mathbf{x},t) = \frac{-i}{\sqrt{\mathcal{D}_0\mathcal{D}^n}} \sum_{\substack{\ell\in\mathbb{Z}\\ \mathbf{m}\in\mathbb{Z}^n}} f(h\mathbf{m},\tau\ell) \int_0^t \psi\Big(\frac{t-\tau\ell-s}{\tau\sqrt{\mathcal{D}_0}}\Big) \int_{\mathbb{R}^n} \frac{\mathrm{e}^{i\,|\mathbf{x}-\mathbf{y}|^2/(4s)}}{(4\pi i s)^{n/2}} \eta\Big(\frac{\mathbf{y}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\Big) d\mathbf{y}\, ds$$

$$= \frac{-i}{\sqrt{\mathcal{D}_0\,\mathcal{D}^n}} \sum_{\substack{\ell\in\mathbb{Z}\\ \mathbf{m}\in\mathbb{Z}^n}} f(h\mathbf{m},\tau\ell) \int_0^t \psi\Big(\frac{t-\tau\ell-s}{\tau\sqrt{\mathcal{D}_0}}\Big) \mathcal{S}\eta\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}, \frac{s}{h^2\mathcal{D}}\Big)\, ds \tag{2.9}$$

where $f(h\mathbf{m},\tau\ell)$ for $\ell<0$ in (2.9) are understood as values of the extended function.

Theorem 2.2. *Let (q,r) be an Schrödinger-admissible pair and $N>(n+1)/\min(q',r')$, $q'=q/(q-1)$, $r'=r/(r-1)$. Suppose that the right-hand side f of the inhomogeneous Schrödinger equation (1.3) satisfies $\partial_t^k\partial_{\mathbf{x}}^{\boldsymbol{\alpha}} f \in L^{r',q'}(\mathbb{R}_+)$ for all $0\le k+|\boldsymbol{\alpha}|\le N$. Then there exist a constant C and for any $\varepsilon>0$ parameters $\mathcal{D}_0,\mathcal{D}>0$, not depending on f, such that the cubature formula (2.9) provides the approximation estimate*

$$\|\Pi f - \Pi_{h,\tau} f\|_{L^{r,q}(\mathbb{R}_+)} \le C \sum_{k=0}^{N} \sum_{|\boldsymbol{\alpha}|=N-k} (\tau\sqrt{\mathcal{D}_0})^k (h\sqrt{\mathcal{D}})^{N-k} \|\partial_t^k\partial_{\mathbf{x}}^{\boldsymbol{\alpha}} f\|_{L^{r',q'}(\mathbb{R}_+)}$$
$$+\,\varepsilon \sum_{k=0}^{N-1}\sum_{j=0}^{N-1-k} \frac{(\tau\sqrt{\mathcal{D}_0})^k (h\sqrt{\mathcal{D}})^j}{(2\pi)^{k+j}} \sum_{|\boldsymbol{\alpha}|=j} \|\partial_t^k\partial_{\mathbf{x}}^{\boldsymbol{\alpha}} f\|_{L^{r',q'}(\mathbb{R}_+)}\,.$$

3 Cubature formulas

3.1 Approximation of $\mathcal{S}g$

For different basis functions η the integrals on the right in (2.3) allow analytic representations. For example, let for $N=2M$

$$\eta(\mathbf{x}) = \eta_N(\mathbf{x}) = \pi^{-n/2}\, L_{M-1}^{(n/2)}(|\mathbf{x}|^2)\,\mathrm{e}^{-|\mathbf{x}|^2}$$

with the generalized Laguerre polynomials

$$L_k^{(\gamma)}(y) = \frac{\mathrm{e}^{\,y} y^{-\gamma}}{k!}\Big(\frac{d}{dy}\Big)^k \Big(\mathrm{e}^{-y} y^{k+\gamma}\Big), \quad \gamma>-1\,.$$

By using the relation ([14, Theorem 3.5])

$$\eta_N(\mathbf{x}) = \pi^{-n/2} \sum_{j=0}^{M-1} \frac{(-1)^j}{j!\,4^j} \Delta^j \mathrm{e}^{-|\mathbf{x}|^2}$$

we obtain the formula

$$\frac{1}{(\pi i t)^{n/2}} \int_{\mathbb{R}^n} \mathrm{e}^{i|\mathbf{x}-\mathbf{y}|^2/t} \eta_N(\mathbf{y}) d\mathbf{y} = \frac{1}{\pi^n (it)^{n/2}} \sum_{j=0}^{M-1} \frac{(-1)^j}{j!\,4^j} \Delta^j \int_{\mathbb{R}^n} \mathrm{e}^{\,i\,|\mathbf{x}-\mathbf{y}|^2/t} \mathrm{e}^{-|\mathbf{y}|^2}\, d\mathbf{y}$$
$$= \frac{1}{\pi^{n/2}(1+it)^{n/2}} \sum_{j=0}^{M-1} \frac{(-1)^j}{j!\,4^j} \Delta^j \mathrm{e}^{-|\mathbf{x}|^2/(1+it)}\,.$$

In view of ([14, (3.15)])

$$\Delta^j \mathrm{e}^{-|\mathbf{x}|^2} = (-1)^j \, j! \, 4^j \mathrm{e}^{-|\mathbf{x}|^2} L_j^{(n/2-1)}(|\mathbf{x}|^2)$$

an approximate solution of (1.1) is given by the analytic formula

$$\mathcal{S}_h g(\mathbf{x},t) = \mathcal{D}^{-n/2} \sum_{\mathbf{m}\in\mathbb{Z}^n} g(h\mathbf{m}) \Phi_N\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}, \frac{4\,t}{h^2\mathcal{D}}\Big)$$

with

$$\Phi_N(\mathbf{x},t) = \frac{\mathrm{e}^{-|\mathbf{x}|^2/(1+i\,t)}}{\pi^{n/2}(1+i\,t)^{n/2}} \sum_{j=0}^{M-1} \frac{1}{(1+i\,t)^j} \, L_j^{(n/2-1)}\Big(\frac{|\mathbf{x}|^2}{1+i\,t}\Big).$$

Another approximation of order $N = 2M$ of the initial function g can be derived by the quasi-interpolant

$$g_h(\mathbf{x}) = \mathcal{D}^{-n/2} \sum_{\mathbf{m}\in\mathbb{Z}^n} g(h\mathbf{m}) \widetilde{\eta_N}\left(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\right)$$

with a basis function in tensor product form

$$\widetilde{\eta_N}(\mathbf{x}) = \prod_{j=1}^n \chi_{2M}(x_j); \quad \chi_{2M}(x_j) = \frac{(-1)^{M-1}}{2^{2M-1}\sqrt{\pi}(M-1)!} \frac{H_{2M-1}(x_j)\mathrm{e}^{-x_j^2}}{x_j}. \tag{3.1}$$

H_k are the Hermite polynomials

$$H_k(x) = (-1)^k \mathrm{e}^{x^2} \Big(\frac{d}{dx}\Big)^k \mathrm{e}^{-x^2}.$$

Then $u(\mathbf{x},t)$ in (1.4) is approximated by

$$\mathcal{S}_h g(\mathbf{x},t) = \mathcal{D}^{-n/2} \sum_{\mathbf{m}\in\mathbb{Z}^n} g(h\mathbf{m}) \widetilde{\Phi_N}\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}, \frac{4\,t}{h^2\mathcal{D}}\Big) \tag{3.2}$$

with

$$\widetilde{\Phi_N}(\mathbf{x},t) = \prod_{j=1}^n \phi_{2M}(x_j,t) = \prod_{j=1}^n \frac{1}{(\pi\,i\,t)^{1/2}} \int_{\mathbb{R}} \mathrm{e}^{\,i(x_j-y)^2/t} \chi_{2M}(y)\,dy\,, \quad t \neq 0. \tag{3.3}$$

From the representation [14, (3.9) and (3.6)]

$$\chi_{2M}(y) = \frac{1}{\sqrt{\pi}} \sum_{\ell=0}^{M-1} \frac{(-1)^\ell}{\ell!\,4^\ell} \frac{\partial^{2\ell}}{\partial y^{2\ell}} \mathrm{e}^{-y^2}$$

we obtain

$$\phi_{2M}(x_j,t) = \frac{1}{\sqrt{\pi}} \sum_{\ell=0}^{M-1} \frac{(-1)^\ell}{\ell!\,4^\ell} \frac{\partial^{2\ell}}{\partial x_j^{2\ell}} \frac{\mathrm{e}^{-x_j^2/(1+i\,t)}}{(1+i\,t)^{1/2}} = \frac{1}{\sqrt{\pi}} \sum_{\ell=0}^{M-1} \frac{\mathrm{e}^{-x_j^2/(1+i\,t)}}{(1+i\,t)^{\ell+1/2}} \, L_\ell^{(-1/2)}\Big(\frac{x_j^2}{1+i\,t}\Big),$$

which in view of

$$L_\ell^{(-1/2)}(y^2) = \frac{(-1)^\ell}{\ell!\,4^\ell} H_{2\ell}(y)$$

gives

$$\widetilde{\Phi_N}(\mathbf{x},t) = \frac{\mathrm{e}^{-|\mathbf{x}|^2/(1+i\,t)}}{\pi^{n/2}(1+i\,t)^{n/2}} \prod_{j=1}^{n} \sum_{\ell=0}^{M-1} \frac{(-1)^\ell}{\ell!\,4^\ell} \frac{1}{(1+i\,t)^\ell} H_{2\ell}\Big(\frac{x_j}{\sqrt{1+i\,t}}\Big). \tag{3.4}$$

Note that the computation of the approximate solution with the summation (3.2) is very efficient if the function $g(\mathbf{x})$ allows a separated representation; that is, within a prescribed accuracy, it can be represented as sum of products of univariate functions

$$g(\mathbf{x}) = \sum_{p=1}^{P} \alpha_p \prod_{j=1}^{n} g_j^{(p)}(x_j) + \mathcal{O}(\varepsilon)\,. \tag{3.5}$$

Then the products of one-dimensional sums

$$\begin{aligned}\mathcal{S}_h g(\mathbf{x},t) &\approx \frac{h^n}{\pi^{n/2}} \sum_{p=1}^{P} \alpha_p \prod_{j=1}^{n} \sum_{m_j\in\mathbb{Z}} g_j^{(p)}(hm_j)\phi_{2M}\left(\frac{x_j-hm_j}{h\sqrt{\mathcal{D}}}, \frac{4\,t}{h^2\mathcal{D}}\right)\\ &= \frac{h^n}{\pi^{n/2}} \sum_{p=1}^{P} \alpha_p \prod_{j=1}^{n} \sum_{m_j\in\mathbb{Z}} g_j^{(p)}(hm_j) \sum_{\ell=0}^{M-1} \frac{(-1)^\ell}{\ell!\,4^\ell} \frac{\mathrm{e}^{-(x_j-hm_j)^2/(h^2\mathcal{D}+4i\,t)}}{(h^2\mathcal{D}+4i\,t)^{\ell+1/2}} H_{2\ell}\left(\frac{x_j-hm_j}{\sqrt{h^2\mathcal{D}+4i\,t}}\right)\end{aligned}$$

provide the approximation of the n-dimensional initial value problem for the Schrödinger equation (1.1).

3.2 Approximation of Πf in (1.5)

Let us assume in (2.8)

$$\psi(t) = \chi_{2M}(t), \qquad \eta(\mathbf{x}) = \prod_{j=1}^{n} \chi_{2M}(x_j).$$

Then Πf is approximated by

$$\begin{aligned}\Pi_{h,\tau} f(\mathbf{x},t) &= \Pi(\mathcal{N}_{h\sqrt{\mathcal{D}},\tau\sqrt{\mathcal{D}_0}} f)(\mathbf{x},t)\\ &= -\frac{i}{\sqrt{\mathcal{D}_0\mathcal{D}^n}} \sum_{\substack{\ell\in\mathbb{Z}\\ \mathbf{m}\in\mathbb{Z}^n}} f(h\mathbf{m},\tau\ell) \int_0^t \chi_{2M}\Big(\frac{s-\tau\ell}{\tau\sqrt{\mathcal{D}_0}}\Big)\, \widetilde{\Phi_N}\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}, \frac{4\,(t-s)}{h^2\mathcal{D}}\Big) ds.\end{aligned} \tag{3.6}$$

The approximation of Πf requires the computation of a certain number of one-dimensional integrals where, for (3.4), the integrands allow separated representations. Suppose that also $f(\mathbf{x},t)$ allows a separated representation, that is

$$f(\mathbf{x},t) = \sum_{p=1}^{P} \beta_p \prod_{j=1}^{n} f_j^{(p)}(x_j,t) + \mathcal{O}(\varepsilon), \tag{3.7}$$

then, for (3.6) and (3.3),

$$\Pi_{h,\tau} f(\mathbf{x},t) \approx \frac{-i}{\sqrt{\mathcal{D}_0\mathcal{D}^n}} \sum_{\ell\in\mathbb{Z}} \sum_{p=1}^{P} \beta_p \int_0^t \chi_{2M}\left(\frac{s-\tau\ell}{\tau\sqrt{\mathcal{D}_0}}\right) \prod_{j=1}^{n} T_j^{(p)}(x_j, \frac{4\,(t-s)}{h^2\mathcal{D}}, \tau\ell) ds \tag{3.8}$$

where

$$T_j^{(p)}(x,t,\tau\ell)=\sum_{m\in\mathbb{Z}} f_j^{(p)}(hm,\tau\ell)\phi_N(\frac{x-hm}{h\sqrt{\mathcal{D}}},t)\,.$$

An accurate quadrature rule of the one-dimensional integrals in (3.8) provides a separated representation of $\Pi_{h,\tau}f$ (this is described in detail in section 4). Then the numerical computation of $\Pi_{h,\tau}f$ does not require to perform n-dimensional integrals and sums but only one-dimensional operations, which leads to a considerable reduction of computing resources, and gives the possibility to treat real world problems.

4 Schrödinger equation over hyper-rectangles

Assume now that g in (1.2) is supported in a hyper-rectangle $[\mathbf{P},\mathbf{Q}]=\{\mathbf{x}\in\mathbb{R}^n : P_j\le x_j\le Q_j, j=1,...,n\}$ and $g\in C^N([\mathbf{P},\mathbf{Q}])$. Hence

$$\mathcal{S}g(\mathbf{x},t)=\frac{1}{(4\pi it)^{n/2}}\int\limits_{[\mathbf{P},\mathbf{Q}]} \mathrm{e}^{i|\mathbf{x}-\mathbf{y}|^2/(4t)}g(\mathbf{y})d\mathbf{y},\quad \mathbf{x}\in\mathbb{R}^n,\quad t\in\mathbb{R} \tag{4.1}$$

provides the solution of (1.1) with the data (1.2).

The direct application of the method described in Section 3 does not give good approximations because the sum

$$\mathcal{D}^{-n/2}\sum_{h\mathbf{m}\in[\mathbf{P},\mathbf{Q}]} g(h\mathbf{m})\eta\left(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\right)$$

approximates g only in a subdomain of $[\mathbf{P},\mathbf{Q}]$. To overcome this difficulty we extend g by using the Hestenes reflection principle into a larger domain with preserved smoothness. If $\widetilde{g}$ is the extension of g, since η is of rapid decay, one can fix $r>0$ such that the quasi-interpolant

$$\mathcal{D}^{-n/2}\sum_{h\mathbf{m}\in\Omega_{rh}} \widetilde{g}(h\mathbf{m})\eta\left(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}\right)$$

approximates g in $[\mathbf{P},\mathbf{Q}]$ with the same error estimate of (2.1). Here $\Omega_{rh}=\prod_{j=1}^n I_j,\ I_j=(P_j-rh\sqrt{\mathcal{D}},Q_j+rh\sqrt{\mathcal{D}})$.

In the following we consider the basis functions in tensor product form (3.1). Then the sum

$$\mathcal{S}_h^{[\mathbf{P},\mathbf{Q}]}g(\mathbf{x},t)=\mathcal{D}^{-n/2}\sum_{\mathbf{m}\in\Omega_{rh}}\widetilde{g}(h\mathbf{m})\widetilde{\Phi}_{2M}^{[\mathbf{P_m},\mathbf{Q_m}]}(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}},\frac{4\,t}{h^2\mathcal{D}}),\quad t\neq 0$$

with $\mathbf{P_m}=(\mathbf{P}-h\mathbf{m})/(h\sqrt{\mathcal{D}})$, $\mathbf{Q_m}=(\mathbf{Q}-h\mathbf{m})/(h\sqrt{\mathcal{D}})$, and

$$\widetilde{\Phi}_{2M}^{[\mathbf{P},\mathbf{Q}]}(\mathbf{x},t)=\frac{1}{(\pi\,i\,t)^{n/2}}\int\limits_{[\mathbf{P},\mathbf{Q}]}\mathrm{e}^{i\,|\mathbf{y}-\mathbf{x}|^2/t}\widetilde{\eta_{2M}}(\mathbf{y})d\mathbf{y}=\prod_{j=1}^n\frac{1}{(\pi\,i\,t)^{1/2}}\int\limits_{P_j}^{Q_j}\mathrm{e}^{i\,(y_j-x_j)^2/t}\chi_{2M}(y_j)dy_j,$$

provides an approximation of (4.1) with the error estimate obtained in Theorem 2.1. $\widetilde{\Phi}_{2M}^{[\mathbf{P},\mathbf{Q}]}(\mathbf{x},4\,t)$ gives the solution of the initial problem

$$i\partial_t v+\Delta_{\mathbf{x}}v=0,\qquad v(\mathbf{x},0)=\prod_{j=1}^n I_{(P_j,Q_j)}(x_j)\chi_{2M}(x_j),\qquad \mathbf{x}\in\mathbb{R}^n,\qquad t\in\mathbb{R}. \tag{4.2}$$

Here $I_{(P_j,Q_j)}$ is the characteristic function of the interval (P_j,Q_j). In [12, Theorem 3.1] we prove

Theorem 4.1. *The solution of the initial value problem (4.2) in $\mathbb{R}^n$ can be expressed by the tensor product*

$$v(\mathbf{x},t)=\prod_{j=1}^{n}\big(\Psi_M(x_j,4\,t,P_j)-\Psi_M(x_j,4\,t,Q_j)\big),$$

where

$$\Psi_M(x,t,y)=\frac{1}{2\sqrt{\pi}}\mathrm{e}^{-x^2/(1+i\,t)}\bigg(\operatorname{erfc}(F(x,i\,t,y))\mathcal{P}_M(x,i\,t)-\frac{\mathrm{e}^{-F^2(x,i\,t,y)}}{\sqrt{\pi}}\mathcal{Q}_M(x,i\,t,y)\bigg) \tag{4.3}$$

with the complementary error function erfc, *the argument function*

$$F(x,t,y)=\sqrt{\frac{t+1}{t}}\Big(y-\frac{x}{t+1}\Big), \tag{4.4}$$

and $\mathcal{P}_M$, $\mathcal{Q}_M$ are polynomials in x of degree $2M-2$ and $2M-3$, respectively:

$$\begin{aligned}
\mathcal{P}_M(x,t)&=\sum_{s=0}^{M-1}\frac{(-1)^s}{s!4^s}\frac{1}{(1+t)^{s+1/2}}H_{2s}\left(\frac{x}{\sqrt{1+t}}\right);\\
\mathcal{Q}_1(x,t,y)&=0,\\
\mathcal{Q}_M(x,t,y)&=2\sum_{k=1}^{M-1}\frac{(-1)^k}{k!\,4^k}\sum_{\ell=1}^{2k}\frac{(-1)^\ell}{t^{\ell/2}}\bigg(H_{2k-\ell}(y)H_{\ell-1}\Big(\frac{y-x}{\sqrt{t}}\Big)\\
&\qquad-\binom{2k}{\ell}H_{2k-\ell}\Big(\frac{x}{\sqrt{1+t}}\Big)\frac{H_{\ell-1}\big(F(t,x,y)\big)}{(1+t)^{k+1/2}}\bigg),\ M>1.
\end{aligned} \tag{4.5}$$

From Theorem 4.1 we deduce the following semi-analytic cubature formula for (4.1) with the error $\mathcal{O}((h\sqrt{\mathcal{D}})^{2M})$

$$\frac{1}{\mathcal{D}^{n/2}}\sum_{\mathbf{m}\in\Omega_{rh}}\widetilde{g}(h\mathbf{m})\prod_{j=1}^{n}\bigg(\Psi_M\Big(\frac{x_j-hm_j}{h\sqrt{\mathcal{D}}},\frac{4\,t}{h^2\mathcal{D}},\frac{P_j-hm_j}{h\sqrt{\mathcal{D}}}\Big)-\Psi_M\Big(\frac{x_j-hm_j}{h\sqrt{\mathcal{D}}},\frac{4\,t}{h^2\mathcal{D}},\frac{Q_j-hm_j}{h\sqrt{\mathcal{D}}}\Big)\bigg).$$

If $\widetilde{g}$ allows a separated representation (3.5) we derive that, at the points of the uniform grid $\{h\mathbf{k},\tau s\}$, the $n-$ dimensional integral (4.1) is approximated by the product of one-dimensional sums

$$\frac{1}{\mathcal{D}^{n/2}}\sum_{p=1}^{P}\alpha_p\prod_{j=1}^{n}S_j^{(p)}(h\mathbf{k},\tau s)$$

where

$$S_j^{(p)}(h\mathbf{k},t)=\sum_{m\in I_j}g_j^{(p)}(hm)\Big(\Psi_M\Big(\frac{k_j-m}{\sqrt{\mathcal{D}}},\frac{4\,t}{h^2\mathcal{D}},\frac{P_j-hm}{h\sqrt{\mathcal{D}}}\Big)-\Psi_M\Big(\frac{k_j-m}{\sqrt{\mathcal{D}}},\frac{4\,t}{h^2\mathcal{D}},\frac{Q_j-hm}{h\sqrt{\mathcal{D}}}\Big)\Big).$$

Suppose now that the source term $f(\mathbf{x},t)$ in (1.3) is supported with respect to $\mathbf{x}$ in the hyper-rectangle $[\mathbf{P},\mathbf{Q}]=\{\mathbf{x}\in\mathbb{R}^n: P_j\le x_j\le Q_j, j=1,...,n\}$ and $f\in C^N([\mathbf{P},\mathbf{Q}]\times\mathbb{R})$. Then, from (1.5),

$$\Pi f(\mathbf{x},t)=-i\int_0^t\frac{ds}{(4\pi is)^{n/2}}\int_{[\mathbf{P},\mathbf{Q}]}\mathrm{e}^{i|\mathbf{x}-\mathbf{y}|^2/(4\,s)}f(\mathbf{y},t-s)d\mathbf{y} \tag{4.6}$$

provides the solution of (1.3) with null initial data. We extend $f(\cdot,t)$ outside $[\mathbf{P},\mathbf{Q}]$ with preserved smoothness and denote by $\widetilde{f}$ its extension. Due to the rapid decay of the generating function $\widetilde{\eta}$, one can fix r and r_0, positive parameters, such that the quasi-interpolant

$$\mathcal{N}^{(r,r_0)}_{h\sqrt{\mathcal{D}},\tau\sqrt{\mathcal{D}_0}} f(\mathbf{x},t) = \frac{1}{\mathcal{D}_0^{1/2}\mathcal{D}^{n/2}} \sum_{\substack{h\mathbf{m}\in\Omega_{rh} \\ \tau\ell\in\widetilde{\Omega}_{r_0\tau}}} \widetilde{f}(h\mathbf{m},\tau\ell)\, \chi_{2M}\left(\frac{t-\tau\ell}{\tau\sqrt{\mathcal{D}_0}}\right) \prod_{j=1}^{n} \chi_{2M}\left(\frac{x_j - hm_j}{h\sqrt{\mathcal{D}}}\right)$$

approximates f for all $\mathbf{x}\in[\mathbf{P},\mathbf{Q}]$ and for all $t\in[-T,T]$, $T>0$, with order $\mathcal{O}((h\sqrt{\mathcal{D}}+\tau\sqrt{\mathcal{D}_0})^N)$. Here $\widetilde{\Omega}_{r_0\tau} = (-T - r_0\tau\sqrt{\mathcal{D}}, T + r_0\tau\sqrt{\mathcal{D}})$. Hence

$$\Pi_{h,\tau} f(\mathbf{x},t) = \frac{-i}{\mathcal{D}_0^{1/2}\mathcal{D}^{n/2}} \sum_{\substack{h\mathbf{m}\in\Omega_{rh} \\ \tau\ell\in\widetilde{\Omega}_{r_0\tau}}} \widetilde{f}(h\mathbf{m},\tau\ell) K_{2M}(\mathbf{x},t,h\mathbf{m},\tau\ell),$$

where

$$K_{2M}(\mathbf{x},t,h\mathbf{m},\tau\ell) = \int_0^t \chi_{2M}\Big(\frac{t-s-\tau\ell}{\tau\sqrt{\mathcal{D}_0}}\Big) \widetilde{\Phi}^{[\mathbf{P_m},\mathbf{Q_m}]}_{2M}\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}, \frac{4\,s}{h^2\mathcal{D}}\Big) ds \tag{4.7}$$

and

$$\widetilde{\Phi}^{[\mathbf{P},\mathbf{Q}]}_{2M}(\mathbf{x},t) = \prod_{j=1}^{n} \big(\Psi_M(x_j,t,P_j) - \Psi_M(x_j,t,Q_j)\big).$$

The integrals in (4.7) cannot be taken analytically. Therefore we use an efficient quadrature based on the classical trapezoidal rule, which is exponentially converging for rapidly decaying smooth functions on the real line. Making the substitution introduced in [17]

$$s = t\varphi(\xi), \qquad \varphi(\xi) = \frac{1}{2}\Big(1 + \tanh\big(\frac{a\pi}{2}\sinh\xi\big)\Big) = \frac{1}{1+\mathrm{e}^{-a\pi\sinh\xi}}\,,$$

with certain positive constant a, K_{2M} transforms to

$$K_{2M}(\mathbf{x},t,h\mathbf{m},\tau\ell) = \frac{\pi a t}{2} \int_{-\infty}^{\infty} \chi_{2M}\Big(\frac{t(1-\varphi(\xi)) - \tau\ell}{\tau\sqrt{\mathcal{D}_0}}\Big) \widetilde{\Phi}^{[\mathbf{P_m},\mathbf{Q_m}]}_{2M}\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}, \frac{4\,t\varphi(\xi)}{h^2\mathcal{D}}\Big)\omega(\xi)d\xi$$

where we denote

$$\omega(\xi) = \frac{\cosh\xi}{1+\cosh(a\pi\sinh\xi)}\,.$$

The trapezoidal rule with step size κ gives for sufficiently large $Q\in\mathbf{N}$

$$K_{2M}(\mathbf{x},t,h\mathbf{m},\tau\ell) \approx \frac{\pi a t\kappa}{2} \sum_{q=-Q}^{Q} \chi_{2M}\Big(\frac{t(1-\varphi(\kappa q)) - \tau\ell}{\tau\sqrt{\mathcal{D}_0}}\Big) \widetilde{\Phi}^{[\mathbf{P_m},\mathbf{Q_m}]}_{2M}\Big(\frac{\mathbf{x}-h\mathbf{m}}{h\sqrt{\mathcal{D}}}, \frac{4\,t\varphi(\kappa q)}{h^2\mathcal{D}}\Big)\omega(q).$$

We obtain that, at the points of the uniform grid $\{h\mathbf{k},\tau s\}$, the $n-$dimensional integral (4.6) is approximated by

$$\Pi_{h,\tau} f(h\mathbf{k},\tau s) \approx \frac{-i\,\pi a\tau s\kappa}{2\mathcal{D}_0^{1/2}\mathcal{D}^{n/2}} \sum_{\substack{h\mathbf{m}\in\Omega_{rh} \\ \tau\ell\in\widetilde{\Omega}_{r_0\tau}}} \widetilde{f}(h\mathbf{m},\tau\ell)$$

$$\times \sum_{q=-Q}^{Q} \chi_{2M}\Big(\frac{s(1-\varphi(\kappa q)) - \ell}{\sqrt{\mathcal{D}_0}}\Big) \widetilde{\Phi}^{[\mathbf{P_m},\mathbf{Q_m}]}_{2M}\Big(\frac{\mathbf{k}-\mathbf{m}}{\sqrt{\mathcal{D}}}, \frac{4\,\tau\ell\varphi(\kappa q)}{h^2\mathcal{D}}\Big)\omega(q).$$

If $\widetilde{f}$ allows a separated representation (3.7) we get the efficient high order approximation

$$\begin{aligned}\Pi_{h,\tau} f(h\mathbf{k},\tau s) \approx & \frac{-i\,\pi a\tau s\kappa}{2\mathcal{D}_0^{1/2}\mathcal{D}^{n/2}} \sum_{q=-Q}^{Q} \omega(q) \\ & \times \sum_{\tau\ell\in\widetilde{\Omega}_{r_0\tau}} \chi_{2M}\Big(\frac{s(1-\varphi(\kappa q))-\ell}{\sqrt{\mathcal{D}_0}}\Big) \sum_{p=1}^{P} \beta_p \prod_{j=1}^{n} T_j^{(p)}(k_j,\tau s,\tau\ell,\kappa q)\,,\end{aligned} \tag{4.8}$$

where

$$\begin{aligned}T_j^{(p)}(k_j,\tau s,\tau\ell,\kappa q) = \sum_{hm_j\in I_j} f_j^{(p)}(hm_j,\tau\ell) \Big(& \Psi_M\Big(\frac{k_j-m_j}{\sqrt{\mathcal{D}}},\frac{4\tau s\varphi(\kappa q)}{h^2\mathcal{D}},\frac{P_j-hm_j}{\sqrt{\mathcal{D}}}\Big) \\ & -\Psi_M\Big(\frac{k_j-m_j}{\sqrt{\mathcal{D}}},\frac{4\tau s\varphi(\kappa q)}{h^2\mathcal{D}},\frac{Q_j-hm_j}{\sqrt{\mathcal{D}}}\Big)\Big)\,.\end{aligned} \tag{4.9}$$

We obtain that, if f has the form (3.7), then the approximation of the potential (4.6) requires us to compute $2QPn$ one-dimensional sums. Thus, if $n>1$, the computational time scales linearly in the space dimension n.

For an efficient implementation of Ψ_M we express erfc in (4.3) with the Faddeeva or scaled complementary error function $W(z)=\mathrm{e}^{-z^2}\operatorname{erfc}(-iz)$ (cf. [3, 7.1.3]) and write

$$\begin{aligned}\Psi_M(x,t,y) &= \frac{\mathrm{e}^{-x^2/(1+it)-F^2(x,it,y)}}{2\sqrt{\pi}}\Big(W\big(iF(x,it,y)\big)\mathcal{P}_M(x,it)-\frac{\mathcal{Q}_M(x,it,y)}{\sqrt{\pi}}\Big) \\ &= \frac{\mathrm{e}^{-y^2+i(y-x)^2/t}}{2\sqrt{\pi}}\Big(W\big(iF(x,it,y)\big)\mathcal{P}_M(x,it)-\frac{\mathcal{Q}_M(x,it,y)}{\sqrt{\pi}}\Big)\,,\end{aligned}$$

where $F(x,it,y)$ is defined by (4.4). Efficient implementations of double precision computations of $W(z)$ are available if the imaginary part of the argument is nonnegative. Otherwise, for $\operatorname{Im} z<0$ overflow problems can occur, which can be seen from the relation $W(z)=2\mathrm{e}^{-z^2}-W(-z)$ (cf. [3, 7.1.11]). But this helps to derive a stable formula also for $\operatorname{Im}(iF(x,it,y))=\operatorname{Re}F(x,it,y)<0$, since

$$\begin{aligned}\frac{\mathrm{e}^{-x^2/(1+it)-F^2(x,it,y)}}{2}W(iF(x,it,y)) &= \frac{\mathrm{e}^{-x^2/(1+it)-F^2(x,it,y)}}{2}\Big(2\mathrm{e}^{F^2(x,it,y)}-W\big(-iF(x,it,y)\big)\Big) \\ &= \mathrm{e}^{-x^2/(1+it)}-\frac{\mathrm{e}^{-y^2+i(y-x)^2/t}}{2}W\big(-iF(x,it,y)\big)\,.\end{aligned}$$

Thus we get the efficient formula

$$\begin{aligned}\Psi_M(x,t,y) =& -\frac{\mathrm{e}^{-y^2+i(y-x)^2/t}}{2\sqrt{\pi}}\frac{\mathcal{Q}_M(x,it,y)}{\sqrt{\pi}} \\ &+\begin{cases}\mathrm{e}^{-y^2+i(y-x)^2/t}\,W\big(iF(x,it,y)\big)\dfrac{\mathcal{P}_M(x,it)}{2\sqrt{\pi}}, & \operatorname{Re}F(x,it,y)\geq 0\,,\\ \Big(2\,\mathrm{e}^{-x^2/(1+it)}-\mathrm{e}^{-y^2+i(y-x)^2/t}\,W\big(-iF(x,it,y)\big)\Big)\dfrac{\mathcal{P}_M(x,it)}{2\sqrt{\pi}}, & \operatorname{Re}F(x,it,y)<0\,.\end{cases}\end{aligned} \tag{4.10}$$

5 Numerical Tests

In this section we present some numerical results. First we verify numerically the accuracy and the convergence order of the proposed method for the inhomogeneous Schrödinger equation (1.3) with null initial data and then for the initial value problem (1.1)-(1.2). Finally, in Figures 2-6, we depict the evolution of $u(\mathbf{x}, t)$ under the two-dimensional equation (1.1) for different initial values.

5.1 Inhomogeneous Schrödinger equation

We consider the Cauchy problem

$$i\frac{\partial u}{\partial t} + \Delta_{\mathbf{x}} u = f(\mathbf{x}, t), \quad u(\mathbf{x}, 0) = 0 \quad \mathbf{x} \in \mathbb{R}^n \tag{5.1}$$

for right hand sides

$$f(\mathbf{x}, t) = \left(i\frac{\partial}{\partial t} + \Delta_{\mathbf{x}}\right) \prod_{j=1}^{n} w(x_j) v(t) \tag{5.2}$$

with $\operatorname{supp} w \subset [-1, 1]$. If $w(\pm 1) = w'(\pm 1) = 0$ and $v(0) = 0$, then the solution of (5.1) is

$$\Pi f(\mathbf{x}, t) = v(t) \prod_{j=1}^{n} w(x_j).$$

If $w \in C^N([p, q])$, we construct a Hestenes extension of $w(x)$ outside $[p, q]$ as

$$\widetilde{w}(x) = \begin{cases} \displaystyle\sum_{s=1}^{N+1} c_s w(-\alpha_s(x-q)+q), & q < x \le q + \dfrac{q-p}{A} \\ w(x), & p \le x \le q \\ \displaystyle\sum_{s=1}^{N+1} c_s w(-\alpha_s(x-p)+p), & p - \dfrac{q-p}{A} \le x < p \end{cases} \tag{5.3}$$

where $\{a_1, ..., a_{N+1}\}$ are different positive constants, $A = \max \alpha_s$, and $\mathbf{c}_N = \{c_1, ..., c_{N+1}\}$ satisfy the system

$$\sum_{s=1}^{N+1} c_s (-\alpha_s)^k = 1, \quad k = 0, ..., N.$$

Hence an extension of $f(\mathbf{x}, t)$ with preserved smoothness is

$$\widetilde{f}(\mathbf{x}, t) = v(t) \prod_{j=1}^{n} \widetilde{w}(x_j)\,.$$

We compare the values of the exact and the approximate solution for (5.1). In all the experiments the approximations have been computed using (4.8)-(4.9) and the function Ψ_M in (4.10). We choose the constants $\mathcal{D} = \mathcal{D}_0 = 4$ to have the saturation error comparable with the double precision rounding errors and the parameters in the quadrature rule $\kappa = 10^{-5}$, $Q = 3{\cdot}10^6$, $a = 1$.

In Tables 1 and 2 we report on the absolute errors and the approximation rates in the space dimensions $n = 1, 3, 10, 20, 100, 200$ for the solution of (5.1) with $v(t) = t$, $w(x) = \cos^2(5\pi x/2)$ and the Hestenes extension obtained by assuming $\alpha_s = 1/s$ (Table 1); $w(x) = \mathrm{e}^{4ix}(x^2-1)^2$ and $\widetilde{w}(x) = w(x)$ (Table 2). The results show that, for high dimensions, the second order fails but the forth and sixth order formulas approximate the exact solution with the predicted approximation rates.

5.2 Initial value problem

Consider the initial value problem

$$i\frac{\partial u}{\partial t} + \Delta_{\mathbf{x}} u = 0, \quad u(\mathbf{x}, 0) = g(\mathbf{x}) = \prod_{j=1}^{n} w(x_j), \quad w(x_j) = 0 \quad \text{if} \quad x_j \notin [-1, 1]. \tag{5.4}$$

Thus $\operatorname{supp} g \subset [-1,1]^n$ and denote by $\widetilde{w}$ the extension of w outside $[-1,1]$ with preserved smoothness. An approximate solution of (5.4) is given by

$$u_h(\mathbf{x},t) = \frac{1}{\mathcal{D}^{n/2}} \prod_{j=1}^{n} \sum_{hm\in I} \widetilde{w}(hm)\Big(\Psi_M\big(\frac{x_j - hm}{h\sqrt{\mathcal{D}}}, \frac{4t}{h^2\mathcal{D}}, \frac{-1-hm}{h\sqrt{\mathcal{D}}}\big) - \Psi_M\big(\frac{x_j - hm}{h\sqrt{\mathcal{D}}}, \frac{4t}{h^2\mathcal{D}}, \frac{1-hm}{h\sqrt{\mathcal{D}}}\big)\Big) \tag{5.5}$$

with $I = (-1 - r\sqrt{\mathcal{D}}, 1 + r\sqrt{\mathcal{D}})$.

In this part we provide results of some experiments which show accuracy and numerical convergence orders. We assume $w(x) = \mathrm{e}^{(x+a)^2}$ which gives the exact solution of (5.4)

$$u(\mathbf{x},t) = \prod_{j=1}^{n} \frac{i\mathrm{e}^{\frac{(a+x_j)^2}{1-4it}}}{2\sqrt{4it-1}} \left(\operatorname{erfc}\left(\frac{4i(a+1)t + x_j - 1}{2\sqrt{t}\sqrt{4t+i}} \right) - \operatorname{erfc}\left(\frac{4i(a-1)t + x_j + 1}{2\sqrt{t}\sqrt{4t+i}} \right) \right)$$

and we compare the calculated solution u_h with the exact solution u. In our experiments we choose $a = 0.32612$. In Figure 1 we report on the absolute error at some grid points in dimensions $n = 1, 3, 10, 50, 100$. The approximations have been computed with $\mathcal{D} = 4$, $M = 3$ and $h = 1/160$ in (5.5), and the Hestenes extension with $\alpha_s = 1/2^s$. If g allows the representation (3.5) that is g has rank P then, denoting by $\varepsilon_j^{(p)}$ the 1-dimensional error for each function $g_j^{(p)}$, then the total error $\varepsilon_n = \mathcal{O}\left(\sum_{p=1}^{P}\sum_{j=1}^{n}\varepsilon_j^{(p)}\right)$. Results in Figure 1 confirm that, for $P = 1$ and g in (5.4), the $n-$dimensional error $\varepsilon_n = \mathcal{O}(n\varepsilon_1)$.

In Table 3 we show that formula (5.5) approximates the exact solution with the predicted approximate orders $N = 2, 4, 6$ in the space dimensions $n = 1, 3, 10, 20, 100, 200$.

We conclude the paper illustrating the evolution of $u(\mathbf{x}, t)$ evolving under the two-dimensional Schrödinger equation (5.4). First we consider the evolvement of the traveling Gaussian $u(\mathbf{x}, 0) = \mathrm{e}^{c\,i(x_1-x_2)}\mathrm{e}^{-60|\mathbf{x}|^2}$ on the domain $(-1.25, 1.25) \times (-1.25, 1.25)$ at four consecutive time values. Figures 2 and 3 show the evolution of $\operatorname{Re} u(\mathbf{x}, t)$ and $|u(\mathbf{x}, t)|$ when $c = 30$. At time $t = 0.04$ the solution has almost completely left the domain. The case $c = 10$ is reported in Figures 4 and 5. Figures 6 and 7 concern the initial data $g(x_1, x_2) = \mathrm{e}^{30\,ix_1}\mathrm{e}^{-60(x_1-1/4)^2}\sin(\pi x_2)$. The figures of the imaginary part of $u(\mathbf{x}, t)$ are virtually the same as for the real part, so we skipped that plots. In all the figures we used the approximation formula of order $N = 6$, the extension of $\widetilde{w}_j = w_j$ and the step $h = 0.005$. Similar tests with finite difference scheme can be found in [2] and [15].

	h^{-1}	τ^{-1}	$M=1$ error	$M=1$ rate	$M=2$ error	$M=2$ rate	$M=3$ error	$M=3$ rate
$n=1$	40	80	0.146E+00		0.326E-01		0.296E-02	
	80	160	0.177E-01	3.04	0.106E-02	4.94	0.248E-04	6.89
	160	320	0.222E-02	2.99	0.313E-04	5.08	0.176E-06	7.13
$n=3$	40	80	0.779E-01		0.135E-01		0.126E-02	
	80	160	0.194E-01	2.00	0.482E-03	4.80	0.103E-04	6.93
	160	320	0.522E-02	1.89	0.240E-04	4.32	0.103E-04	6.93
$n=10$	40	80	0.243E+00		0.236E-01		0.122E-02	
	80	160	0.789E-01	1.62	0.163E-02	3.86	0.208E-04	5.87
	160	320	0.212E-01	1.89	0.104E-03	3.97	0.356E-06	5.87
$n=20$	40	80	0.378E+00		0.486E-01		0.258E-02	
	80	160	0.152E+00	1.31	0.343E-02	3.82	0.441E-04	5.87
	160	320	0.436E-01	1.80	0.219E-03	3.97	0.771E-06	5.84
$n=100$	40	80	0.500E+00		0.207E+00		0.133E-01	
	80	160	0.424E+00	0.23	0.176E-01	3.55	0.230E-03	5.85
	160	320	0.189E+00	1.16	0.114E-02	3.95	0.402E-05	5.84
$n=200$	40	80	0.500E+00		0.329E+00		0.264E-01	
	80	160	0.489E+00	0.03	0.348E-01	3.24	0.462E-03	5.84
	160	320	0.308E+00	0.66	0.229E-02	3.92	0.778E-05	5.89

Table 1: Absolute errors and approximation rates for the solution of (5.1) with $f(\mathbf{x},t)$ in (5.2) where $w(x) = \cos^2(5\pi x/2)$ and $v(t) = t$, at the point $\mathbf{x} = (0.1, 0.4, ..., 0.4)$; $t = 1$ using formula (4.8)-(4.9) with (4.10) and the Hestenes extension corresponding to $\alpha_s = 1/s$.

	h^{-1}	τ^{-1}	$M=1$ error	$M=1$ rate	$M=2$ error	$M=2$ rate	$M=3$ error	$M=3$ rate
$n=1$	20	40	0.638E-01		0.153E-02		0.724E-04	
	40	80	0.162E-01	1.98	0.986E-04	3.96	0.122E-05	5.89
	80	160	0.407E-02	1.99	0.621E-05	3.99	0.199E-07	5.94
$n=3$	20	40	0.133E+00		0.550E-02		0.168E-03	
	40	80	0.354E-01	1.96	0.361E-03	3.93	0.277E-05	5.92
	80	160	0.899E-02	1.97	0.228E-04	3.98	0.439E-07	5.98
$n=10$	20	40	0.321E+00		0.161E-01		0.512E-03	
	40	80	0.968E-01	1.73	0.106E-02	3.92	0.843E-05	5.92
	80	160	0.254E-01	1.92	0.672E-04	3.98	0.134E-06	5.98
$n=20$	20	40	0.423E+00		0.260E-01		0.837E-03	
	40	80	0.149E+00	1.50	0.174E-02	3.91	0.138E-04	5.92
	80	160	0.409E-01	1.86	0.110E-03	3.98	0.219E-06	5.98
$n=100$	20	40	0.133E+00		0.242E-01		0.836E-03	
	40	80	0.964E-01	0.46	0.173E-02	3.80	0.138E-04	5.92
	80	160	0.363E-01	1.41	0.110E-03	3.97	0.219E-06	5.98
$n=200$	20	40	0.180E-01		0.590E-02		0.223E-03	
	40	80	0.166E-01	0.11	0.461E-03	3.68	0.370E-05	5.91
	80	160	0.843E-02	0.97	0.295E-04	3.97	0.587E-07	5.98

Table 2: Absolute errors and approximation rates for the solution of (5.1) with $f(\mathbf{x},t)$ in (5.2) where $w(x) = e^{4ix}(x^2-1)^2$ and $v(t) = t$, at the point $\mathbf{x} = (0.1, 0.1, ..., 0.1)$; $t = 1$ using formula (4.8)-(4.9) with (4.10) and the extension $\widetilde{w}(x) = w(x)$.

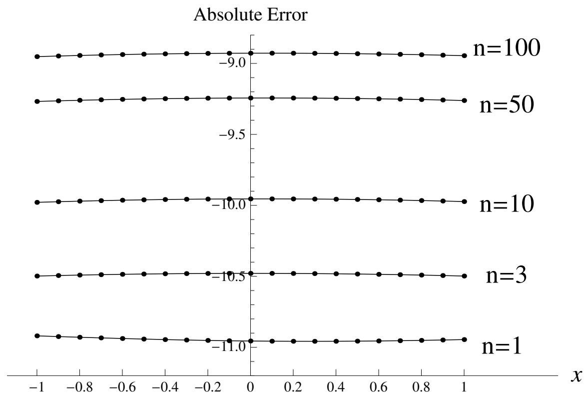

Figure 1: Absolute errors, using $\log_{10}$ scale on the vertical axes, for the solution of (5.4) with $w(x) = \mathrm{e}^{(x+a)^2}$, $a = 0.32612$, the Hestenes extension corresponding to $\alpha_s = 1/2^s$, using (5.5) with $h = 1/160$, $\mathcal{D} = 4$, $\mathbf{x} = (x, 0.1, ..., 0.1)$, $t = 1$.

	h^{-1}	$M = 1$ error	rate	$M = 2$ error	rate	$M = 3$ error	rate
$n = 1$	40	3.069E-03		1.178E-05		4.522E-08	
	80	7.693E-04	1.99	7.438E-07	3.98	7.206E-10	5.97
	160	1.924E-04	1.99	4.661E-08	3.99	1.151E-11	5.96
	320	4.812E-05	1.99	2.915E-09	3.99	2.158E-13	5.73
$n = 3$	40	9.246E-03		3.538E-05		1.357E-07	
	80	2.312E-03	1.99	2.233E-06	3.98	2.163E-09	5.97
	160	5.781E-04	1.99	1.399E-07	3.99	3.457E-11	5.96
	320	1.445E-04	1.99	8.754E-09	3.99	6.455E-13	5.74
$n = 10$	40	1.292E-01		1.184E-04		4.546E-07	
	80	7.764E-03	2.01	7.479E-06	3.98	7.246E-09	5.97
	160	1.937E-03	2.00	4.687E-07	3.99	1.157E-10	5.96
	320	4.840E-04	2.00	2.931E-08	3.99	2.159E-12	5.74
$n = 20$	40	6.400E-02		2.385E-04		9.155E-07	
	80	1.569E-02	2.02	1.505E-05	3.98	1.458E-08	5.97
	160	3.904E-03	2.00	9.437E-07	3.99	2.331E-10	5.96
	320	9.749E-04	2.00	5.902E-08	3.99	4.347E-12	5.74
$n = 100$	40	3.832E-01		1.258E-03		4.831E-06	
	80	8.542E-02	2.16	7.947E-05	3.98	7.700E-08	5.97
	160	2.076E-02	2.04	4.980E-06	3.99	1.230E-09	5.96
	320	5.155E-03	2.01	3.115E-07	3.99	2.294E-11	5.74
$n = 200$	40	9.669E-01		2.691E-03		1.033E-05	
	80	1.901E-01	2.34	1.700E-04	3.98	1.647E-07	5.97
	160	4.486E-02	2.08	1.065E-05	3.99	2.632E-09	5.96
	320	1.105E-02	2.02	6.665E-07	3.99	4.908E-11	5.74

Table 3: Absolute errors and approximation rates for the solution of (5.4) with $w(x) = \mathrm{e}^{(x+a)^2}$, $a = 0.32612$, at the point $\mathbf{x} = (0.2, 0.1, ..., 0.1)$; $t = 1$ using formula (5.5) and the Hestenes extension corresponding to $\alpha_s = 1/s$.

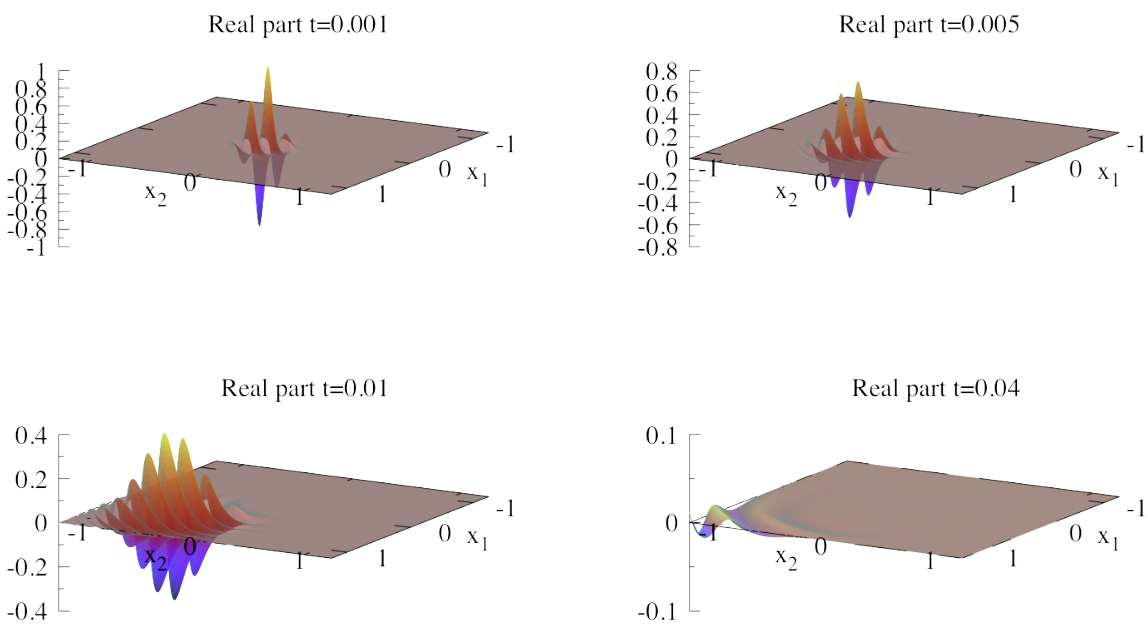

Figure 2: Real part of u when $w_j(x) = \mathrm{e}^{ic_j x}\mathrm{e}^{-60x^2}$, $j = 1, 2$, $c_1 = 30$, $c_2 = -30$, $N = 6$, $h = 0.005$.

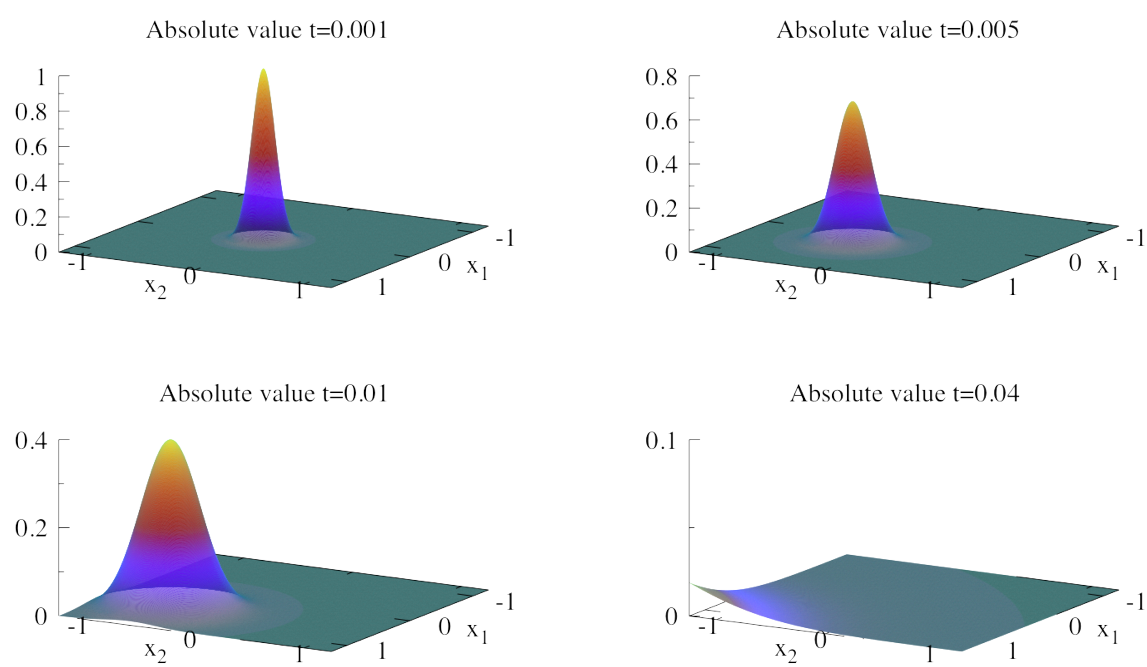

Figure 3: Absolute value of u when $w_j(x) = \mathrm{e}^{ic_j x}\mathrm{e}^{-60x^2}$, $j = 1, 2$, $c_1 = 30$, $c_2 = -30$, $N = 6$, $h = 0.005$.

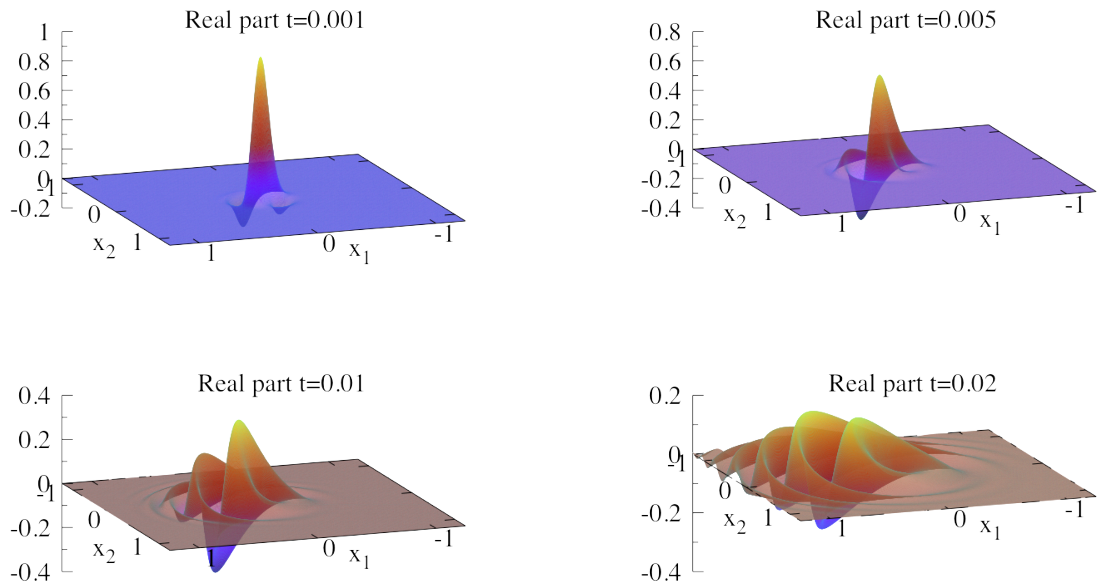

Figure 4: Real part of u when $w_j(x) = \mathrm{e}^{ic_j x}\mathrm{e}^{-60x^2}$, $j = 1, 2$, $c_1 = 10$, $c_2 = -10$, $N = 6$, $h = 0.005$.

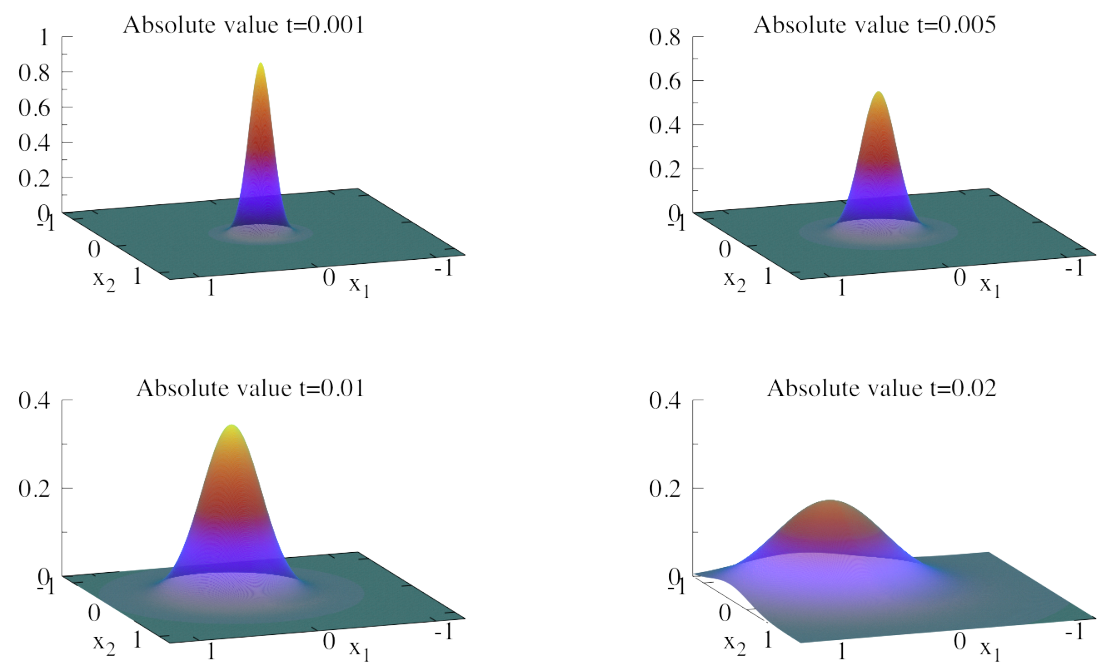

Figure 5: Absolute value of u when $w_j(x) = \mathrm{e}^{ic_j x}\mathrm{e}^{-60x^2}$, $j = 1, 2$, $c_1 = 10$, $c_2 = -10$, $N = 6$, $h = 0.005$

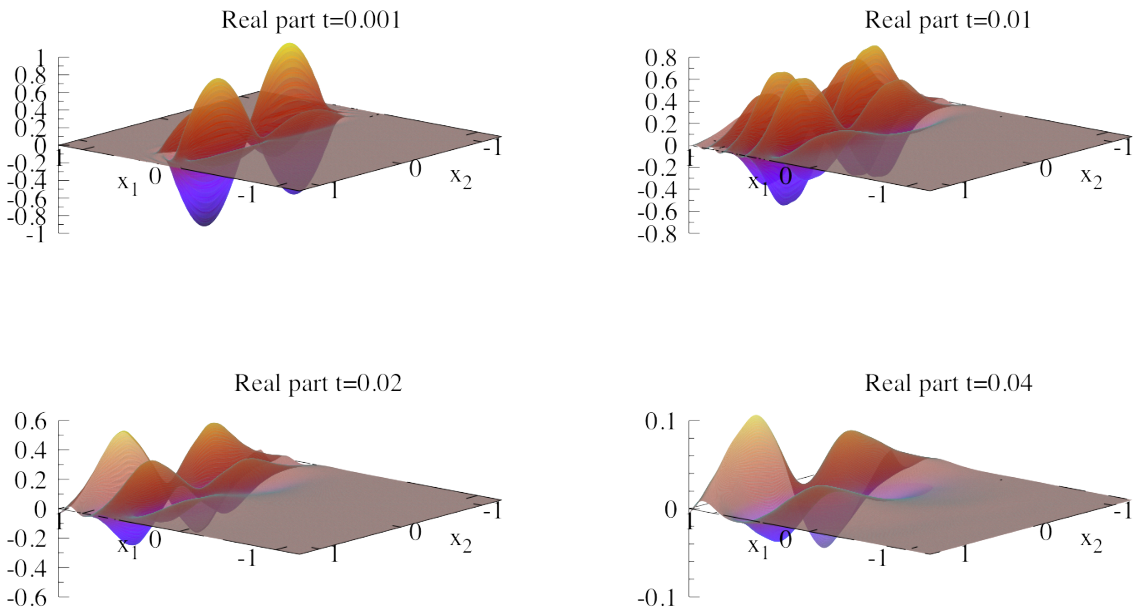

Figure 6: Real part of u when $w_1(x) = \mathrm{e}^{30ix}\mathrm{e}^{-60(x-1/4)^2}$, $w_2(x) = \sin(\pi x)$, $N = 6$, $h = 0.005$.

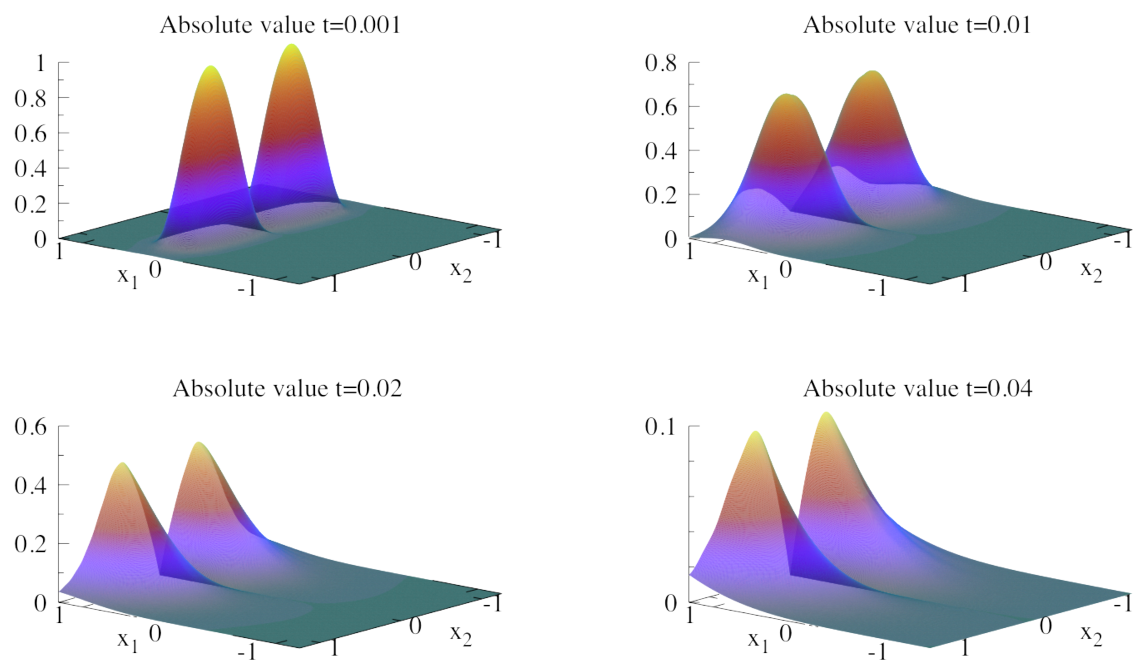

Figure 7: Absolute value of u when $w_1(x) = \mathrm{e}^{30ix}\mathrm{e}^{-60(x-1/4)^2}$, $w_2(x) = \sin(\pi x)$, $N = 6$, $h = 0.005$.

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