Skaičiavimo metodų ir matematinio modeliavimo seminaras Nr. 14 (121)

Apie Šredingerio lygčių su laidžiomis kraštinėmis sąlygomis skaitinį sprendimą

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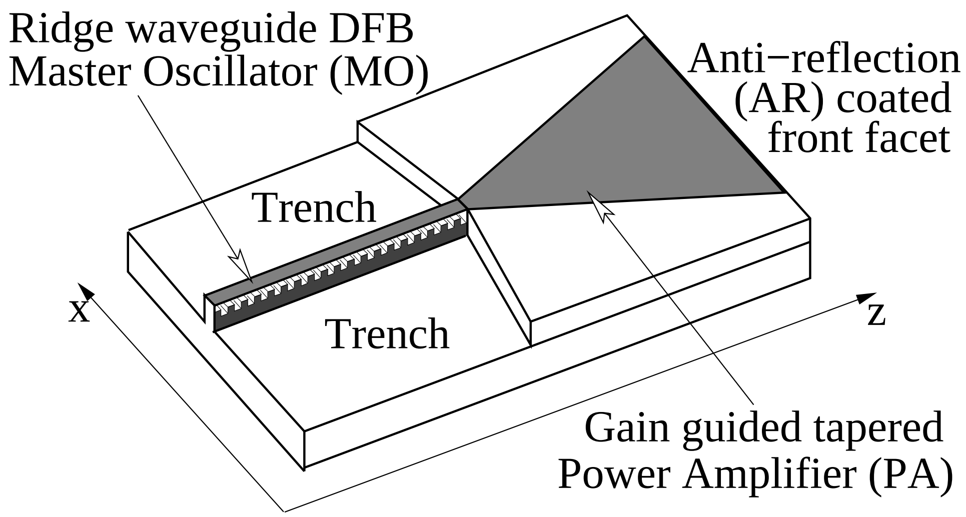
Motivation

A schematic view of a MOPA device:



PROBLEM FORMULATION

Consider the pure initial value problem for the 1D Schrö-dinger equation ($i = \sqrt{-1}$):

$$\frac{\partial \tilde{u}}{\partial t} + iD_f \frac{\partial^2 \tilde{u}}{\partial x^2} - iV(x)\tilde{u} = 0, \quad x \in \mathcal{R},\ t > 0, \quad (1)$$

$$\tilde{u}(x, 0) = u_0(x), \quad x \in \mathcal{R},$$

· Initial data $u_0(x)$ is supported only on some finite domain;

· $V(x) = 0$ for $|x| \leq X_\delta$.

The domain of interest is restricted to a bounded interval $\Omega_x = [-\tilde{X}, \tilde{X}]$.

Our goal is to formulate artificial BCs on an extended interval $(-X, X)$ with $X > \tilde{X}$ as close to $\tilde{X}$ as possible, such that the solution $u(x,t)$ of problem

$$\frac{\partial u}{\partial t} + iD_f \frac{\partial^2 u}{\partial x^2} + \big(\alpha(x) - iV(x)\big)u = 0, \qquad (2)$$
$$u(x,0) = u_0(x), \quad x \in [-X, X],$$
$$F_L u(-X,t) = 0, \quad F_R u(X,t) = 0, \quad t > 0$$

is close to the exact solution of (1), e.g. it satisfies the estimate

$$\int_0^T \int_{-\tilde{X}}^{\tilde{X}} |\tilde{u}(x,t) - u(x,t)|^2 \, dx dt \leq \varepsilon^2.$$

BC ?

$$u(x,t) = \frac{1}{\sqrt{1 - i\frac{t}{\alpha}}} e^{\left[-ik(x-kt) - \frac{(x-2kt)^2}{4(\alpha - it)}\right]}$$

In the case of a parabolic problem the following BCs are used:

1. $u(-X,t) = 0, \quad u(X,t) = 0.$

2. $u'_x(-X,t) = 0, \quad u'_x(X,t) = 0.$

3. $-du'_x(-X,t) + \beta u(-X,t) = g_0.$

Reflective boundary conditions

Let us solve problem (2) in a sufficiently large domain with the reflective BCs:

$$u(-X,t) = 0, \quad u(X,t) = 0, \quad t > 0. \tag{3}$$

For functions $u, v \in L_2(\Omega_x)$ we define the inner product (u, v) and the L_2 norm $\|u\|$ by

$$(u,v) = \int_{-X}^{X} u(x)v^*(x)\,dx, \quad \|u\| = \sqrt{(u,u)}.$$

Let us define mass M and energy E of the solution as

$$M(t) = \int_{-X}^{X} |u(x,t)|^2\,dx,$$

$$E(t) = \int_{-X}^{X} \left(D_f \left| \frac{\partial u}{\partial x}(x,t) \right|^2 + V(x)\,|u(x,t)|^2 \right) dx.$$

Lemma 1. *If* $\alpha(x) \geq 0$ *(or* $\alpha(x) \equiv 0$*) and* $u(x,t)$ *is the solution of problem (2) – (3), then the total mass of the solution is not increased (conserved) in time:*

$$M(t) \equiv \|u(\cdot,t)\|^2 \leq \|u_0\|^2 \equiv M(0) \tag{4}$$

$$(\,\|u(\cdot,t)\|^2 = \|u_0\|^2\,)$$

If $\alpha(x) \equiv 0$ *(i.e. the potential function is real valued), then energy* $E(t)$ *of problem (2) – (3) is conserved:*

$$E(t) = E(0). \tag{5}$$

Proof. Computing the inner product of equation (2) with $u(x,t)$, integrating by parts the diffraction operator and taking the real part of the obtained equality we get the equation

$$\frac{d}{dt}\|u(\cdot,t)\|^2 + 2\int_{-X}^{X} \alpha(x)\,|u(x,t)|^2\,dx = 0.$$

In order to prove (5) we compute the inner product of equation (2) with $\dfrac{\partial}{\partial t}u(x,t)$, integrate by parts the diffraction operator and take the imaginary part of the the obtained equality

$$\frac{\partial}{\partial t}\left(D_f\left\|\frac{\partial u}{\partial x}(\cdot,t)\right\|^2+\int_{-X}^{X}V(x)\,|u(x,t)|^2\,dx\right)$$
$$=2\int_{-X}^{X}\alpha(x)\,\mathrm{Im}\left(u\frac{\partial u^*}{\partial t}\right)\,dx.$$

Thus the absorbtion disturbes the conservativity of the energy $E(t)$.

If $\alpha\equiv 0$, then we get the energy conservation law $\frac{d}{dt}E(t)=0$.

It is easy to get estimates of the solution in the maximum norm:

$$\|u(\cdot,t)\|_\infty = \max_{-X\le x\le X} |u(x,t)|.$$

Lemma 2. *Let* $u(x,t)$ *be the solution of problem (2) – (3). If* $\alpha(x) = 0$ *and* $V(x) \ge 0$ *then* $u(x,t)$ *is bounded unconditionally in the maximum norm*

$$\|u(\cdot,t)\|_\infty \le \sqrt{\frac{XE(0)}{2D_f}}.$$

If $-V_M \le V(x) \le 0$, *then a similar estimate is valid for sufficiantly small* V_M, *i.e. when*

$$\frac{4V_M X^2}{\pi^2} \le qD_f \quad \text{for} \quad q < 1.$$

Proof. If $V(x) \geq 0$, then we have the estimate

$$\left\| \frac{\partial u}{\partial x}(\cdot, t) \right\|^2 \leq \frac{1}{D_f} E(0).$$

It is sufficient to apply the Sobolev imbedding inequality:

$$\|u(\cdot, t)\|_\infty \leq \frac{\sqrt{2X}}{2} \left\| \frac{\partial u}{\partial x}(\cdot, t) \right\|.$$

If $-V_M \leq V(x) \leq 0$, then we use the Sobolev imbedding inequality

$$\|u(\cdot, t)\|^2 \leq \frac{4X^2}{\pi^2} \left\| \frac{\partial u}{\partial x}(\cdot, t) \right\|^2$$

and obtain the inequality

$$D_f \left\| \frac{\partial u}{\partial x}(\cdot, t) \right\|^2 + \int_{-X}^{X} V(x) |u(x, t)|^2 \, dx \geq \left(D_f - V_M \frac{4X^2}{\pi^2} \right) \left\| \frac{\partial u}{\partial x}(\cdot, t) \right\|^2.$$

Absorbing boundary conditions

Let us consider right/left moving single waves

$$u(x,t) = e^{\mp ikx} e^{i\omega t},$$

where $\omega(k)$ denotes the wave frequency and k is the wave number.

Next we use the relation

$$\frac{\partial u}{\partial x} = \mp iku$$

and get the following absorbing boundary conditions

$$-iD_f \frac{\partial u}{\partial x}(-X,t) = \gamma u(-X,t), \qquad (6)$$

$$iD_f \frac{\partial u}{\partial x}(X,t) = \gamma u(X,t),$$

If $\gamma = \frac{1}{2}|v|$, where v is the group velocity of the wave:

$$v := \frac{\partial \omega}{\partial k} = 2D_f k,$$

then the absorbing BCs are exact.

Lemma 3. *Let $\alpha(x) \equiv 0$ and $u(x,t)$ is the solution of problem (2), (6), then the total mass of the solution is not increased in time:*

$$M(t) \equiv \|u(\cdot,t)\|^2 \leq \|u_0\|^2 \equiv M(0). \tag{7}$$

The energy $E(t)$ of the solution satisfies the following conservation equation

$$\frac{\partial}{\partial t}\left(D_f \left\|\frac{\partial u}{\partial x}(\cdot,t)\right\|^2 + \int_{-X}^{X} V(x)\,|u(x,t)|^2\,dx\right) \tag{8}$$
$$= 2\gamma\left(\mathrm{Im}\left(u\frac{\partial u^*}{\partial t}(-X,t)\right) + \mathrm{Im}\left(u\frac{\partial u^*}{\partial t}(X,t)\right)\right).$$

Proof. Computing the inner product of equation (2) with $u(x,t)$, integrating by parts the diffraction operator, using boundary conditions (6) and taking the real part of the obtained equality we get the equation

$$\frac{d}{dt}\|u(\cdot,t)\|^2 + 2\gamma\left(|u(-X,t)|^2 + |u(X,t)|^2\right) = 0.$$

In general, waves are composed of more than one component with different group velocities.

$$\prod_{j=1}^{p} \left(iD_f \frac{\partial}{\partial x} - \gamma_j \right) u \bigg|_{x=X} = 0.$$

How to select optimal values of γ_j ?

Transparent boundary conditions

The original domain is divided into three subproblems Transparent boundary conditions are obtained by using the assumption that at the exterior domains the solution decreases to zero as $|x| \to \infty$ and the potentials are equal to zero.

Exterior problems can be solved explicitly by the Laplace method. We get the following boundary conditions:

$$iD_f \frac{\partial u}{\partial x}\left(-X,t\right) = i\sqrt{\frac{D_f}{\pi}} e^{i\frac{\pi}{4}} \frac{d}{dt} \int_0^t \frac{u(-X,s)}{\sqrt{t-s}}\, ds, \quad (9)$$

$$-iD_f \frac{\partial u}{\partial x}\left(X,t\right) = i\sqrt{\frac{D_f}{\pi}} e^{i\frac{\pi}{4}} \frac{d}{dt} \int_0^t \frac{u(X,s)}{\sqrt{t-s}}\, ds.$$

We note that the nonlocal operator on the right hand side defines a fractional time derivative

$$\sqrt{\frac{d}{dt}}\, v(t) := \frac{1}{\sqrt{\pi}} \frac{d}{dt} \int_0^t \frac{v(s)}{\sqrt{t-s}}\, ds.$$

These derivatives arise in a formal factorization of the Schrödinger equation into left and right travelling waves:

$$\left(\frac{\partial}{\partial x} - \frac{e^{i\pi/4}}{\sqrt{D_f}}\sqrt{\frac{\partial}{\partial t}}\right)\left(\frac{\partial}{\partial x} + \frac{e^{i\pi/4}}{\sqrt{D_f}}\sqrt{\frac{\partial}{\partial t}}\right) u(x,t) = 0.$$

Approximation of nonlocal exact BCs with a sequence of local operators by using rational functions

$$iD_f\frac{\partial u}{\partial x}\big(X,t\big) = \beta_m u(X,t)$$
$$+\sum_{k=1}^{m} a_{km}\Big(u(X,t) - d_{km}\varphi_{km}(t)\Big), \quad m \geq 1,$$

where φ_{km} is defined by

$$\begin{cases} \dfrac{d\varphi_{km}}{dt} + i\Big(d_{km}\varphi_{km}(t) - D_f u(t)\Big) = 0, \quad t > 0, \\ \varphi_{km}(0) = 0. \end{cases}$$

The reflection coefficient is optimized in the L^2 norm with the weight $1/\big(1+(D_f r)^2\big)$

$$\int_0^{T/2\pi}\left|\frac{\sqrt{D_f r} - \beta_m r - \sum_{k=1}^{m}\left(a_{km}r/(1+d_{km}r)\right)}{\sqrt{D_f r} + \beta_m r + \sum_{k=1}^{m}\left(a_{km}r/(1+d_{km}r)\right)}\right|^2 \frac{dr}{1+(D_f r)^2}.$$

Finite-Difference Schemes

We introduce a uniform mesh in x on the interval $[-X, X]$:

$$\bar{\omega}_h = \{x_j : \ x_j = -X + jh, \ j = 0, \dots, J, \ x_J = X\}$$

and a uniform mesh in t on the interval $[0, T]$:

$$\bar{\omega}_\tau = \{t^n : \quad t^n = n\tau, \quad n = 0, \dots, N, \quad t^N = T\}.$$

Let us define discrete functions:

$$U_j^n = U(x_j, t^n), \quad (x_j, t^n) \in \bar{\omega}_h \times \bar{\omega}_\tau.$$

We define the forward and backward difference quotents with respect to x and the backward difference quotent, the symmetric averaging operator in time

$$\partial_x U_j := \frac{U_{j+1} - U_j}{h}, \quad \bar{\partial}_x U_j := \frac{U_j - U_{j-1}}{h},$$

$$\bar{\partial}_t U^n := \frac{U^{n+1} - U^n}{\tau}, \quad U^{n-1/2} := \frac{U^n + U^{n-1}}{2}.$$

We investigate the standard Crank-Nicolson approximation of the Schrōdinger equation (2). Let us consider the reflective BCs:

$$
\begin{cases}
\bar{\partial}_t U_j^n + iD_f \partial_x \bar{\partial}_x U_j^{n-\frac{1}{2}} + (\alpha_j - iV_j) U_j^{n-\frac{1}{2}} = 0, \\
\qquad (x_j, t^n) \in \omega_h \times \omega_\tau, \\
U_0^n = 0, \quad U_J^n = 0, \quad t^n \in \omega_\tau, \\
U_j^0 = u_0(x_j), \quad x_j \in \bar{\omega}_h.
\end{cases}
\tag{10}
$$

Let us introduce some mesh counterparts of the inner products and the norms in the discrete $L_2(\omega_h)$ and $L_2(\bar{\omega}_h)$ spaces:

$$(U,W)_{\omega_h} = \sum_{j=1}^{J-1} U_j V_j^* h,$$

$$(U,W)_{\bar{\omega}_h} = \sum_{j=1}^{J-1} U_j V_j^* h + \frac{h}{2}\Big(U_0 W_0^* + U_J W_J^*\Big),$$

$$\|U\|_D^2 = (U,U)_D.$$

We also define the discrete analogs of mass and energy of discrete problem (10) as

$$M_h^n = \|U^n\|_{\omega_h}^2, \quad E_h^n = \sum_{j=1}^{J} D_f \big|\bar{\partial}_x U_j^n\big|^2 h + (VU^n, U^n)_{\omega_h}.$$

Theorem 1 *If* $\alpha(x) \geq 0$ *(or* $\alpha(x) \equiv 0$*) and* U^n *is the solution of finite-difference scheme (10), then the discrete total mass of the solution is not increased (conserved) in time:*

$$M_h^n \leq M_h^{n-1} \leq \ldots \leq M_h^0, \tag{11}$$
$$(M_h^n = M_h^{n-1} = \ldots = M_h^0).$$

If $\alpha(x) \equiv 0$ *(i.e. the potential function is real valued), then the discrete energy* E_h^n *of (10) is conserved:*

$$E_h^n = E_h^{n-1} = \ldots = E_h^0. \tag{12}$$

Proof.

$$\|U^n\|^2_{\omega_h} + 2(\alpha\, U^{n-1/2}, U^{n-1/2})_{\omega_h} = \|U^{n-1}\|^2_{\omega_h}.$$

We solve the initial-boundary value problem (2) – (3) in the simple case $V(x) \equiv 0$, $D_f = 1$. First, let us set $\alpha(x) \equiv 0$.

We use the standard example of the Gaussian solution

$$u(x,t) = \frac{1}{\sqrt{1 - it/w_0}} \exp\left[-ik(x - kt) - \frac{(x - 2kt)^2}{4(w_0 - it)}\right].$$

We take the following values of parameters: $w_0 = 0.15$, $k = 2$, the domain of interest is defined as $[-2, 2]$, i.e. $X_0 = 2$. Both effects, the diffraction and linear transport with the wave number k, are important in this example.

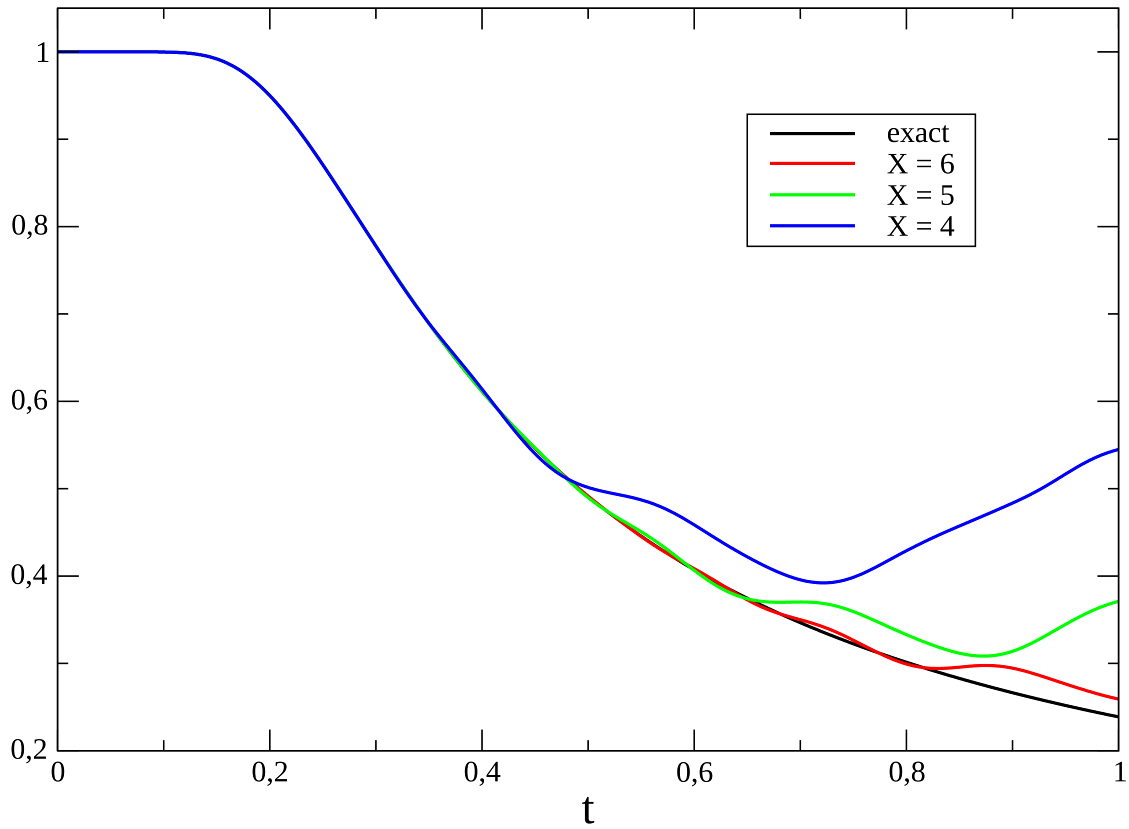
The reflection ratio at time t^n is calculated as

$$r^n = \frac{\sum_{j=s}^{f} |U_j^n|^2}{\sum_{j=s}^{f} |U_j^0|^2}, \quad x_s = -X^0, \;\; x_f = X^0.$$

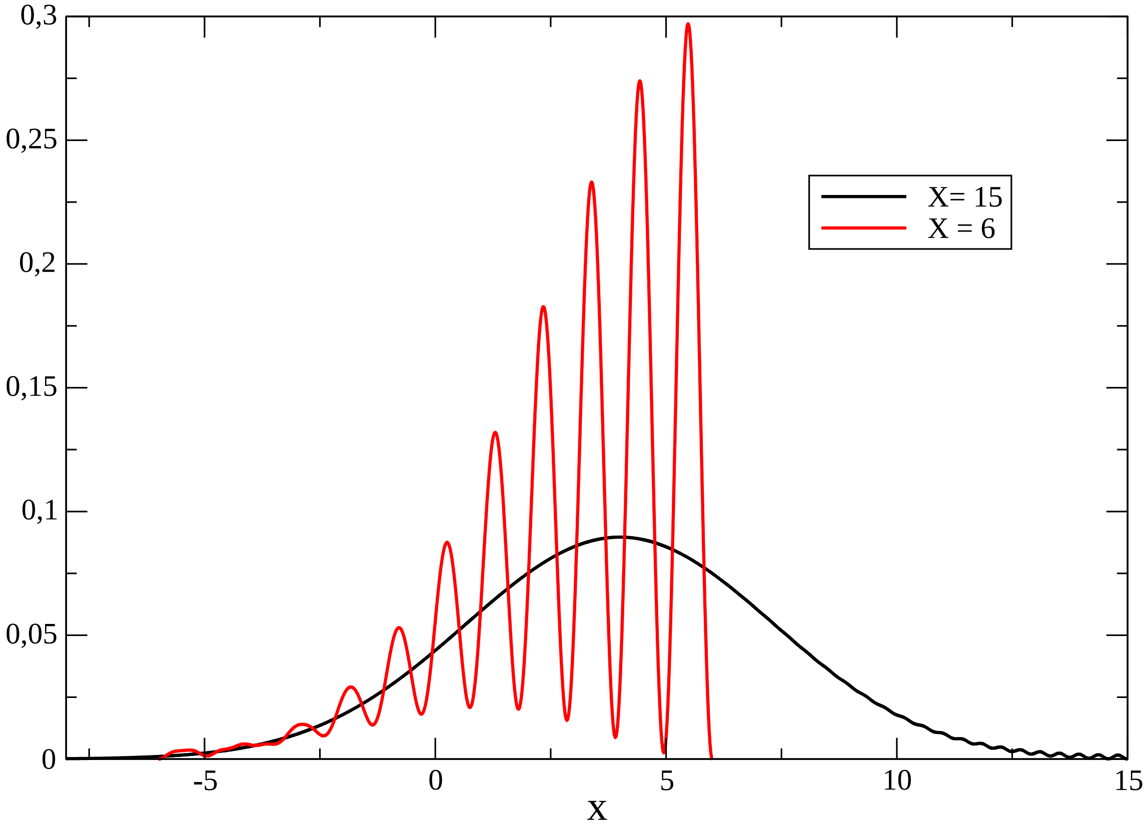
Results of Numerical Experiments

The solution of the finite-difference scheme (10) is computed for $0 \le t \le 1$ with different lengths of the extended domain $X = 4, 5, 6$.

The reflection coefficient.



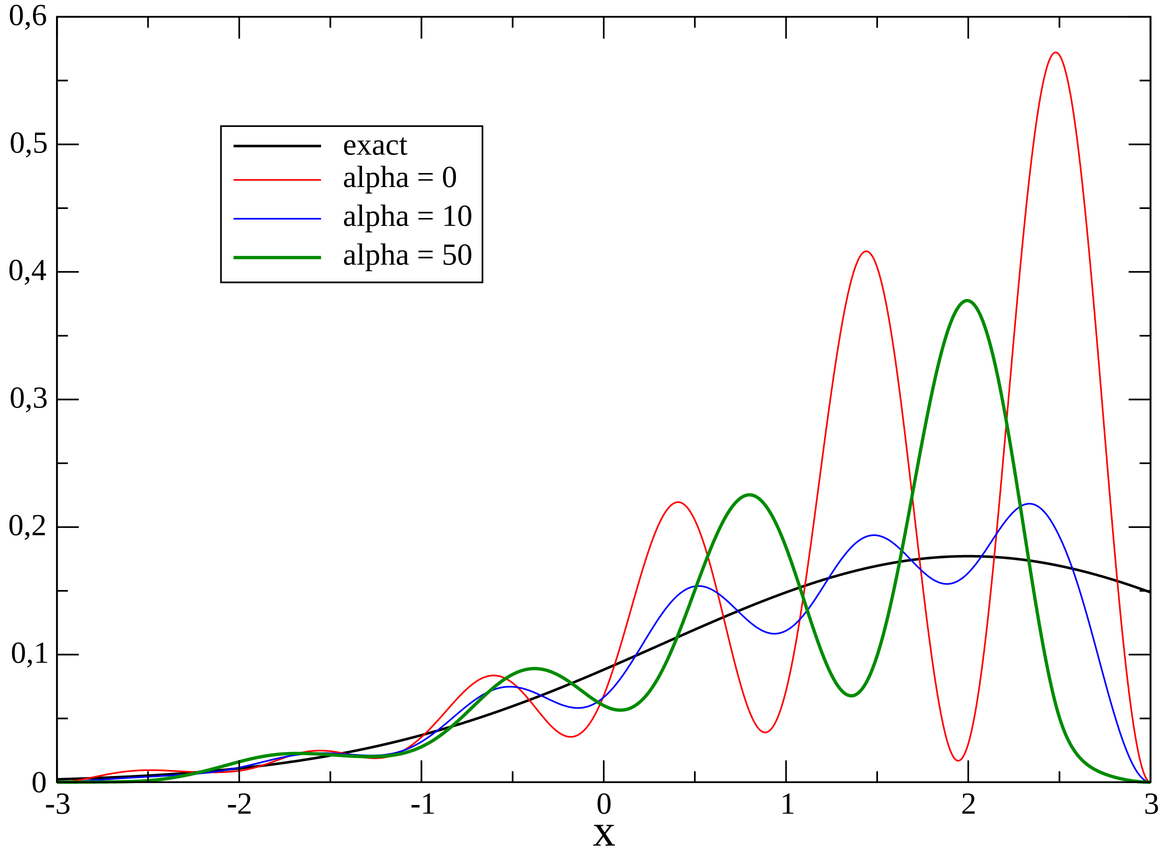
A plot of function $|U(x_j, 1)|^2$.



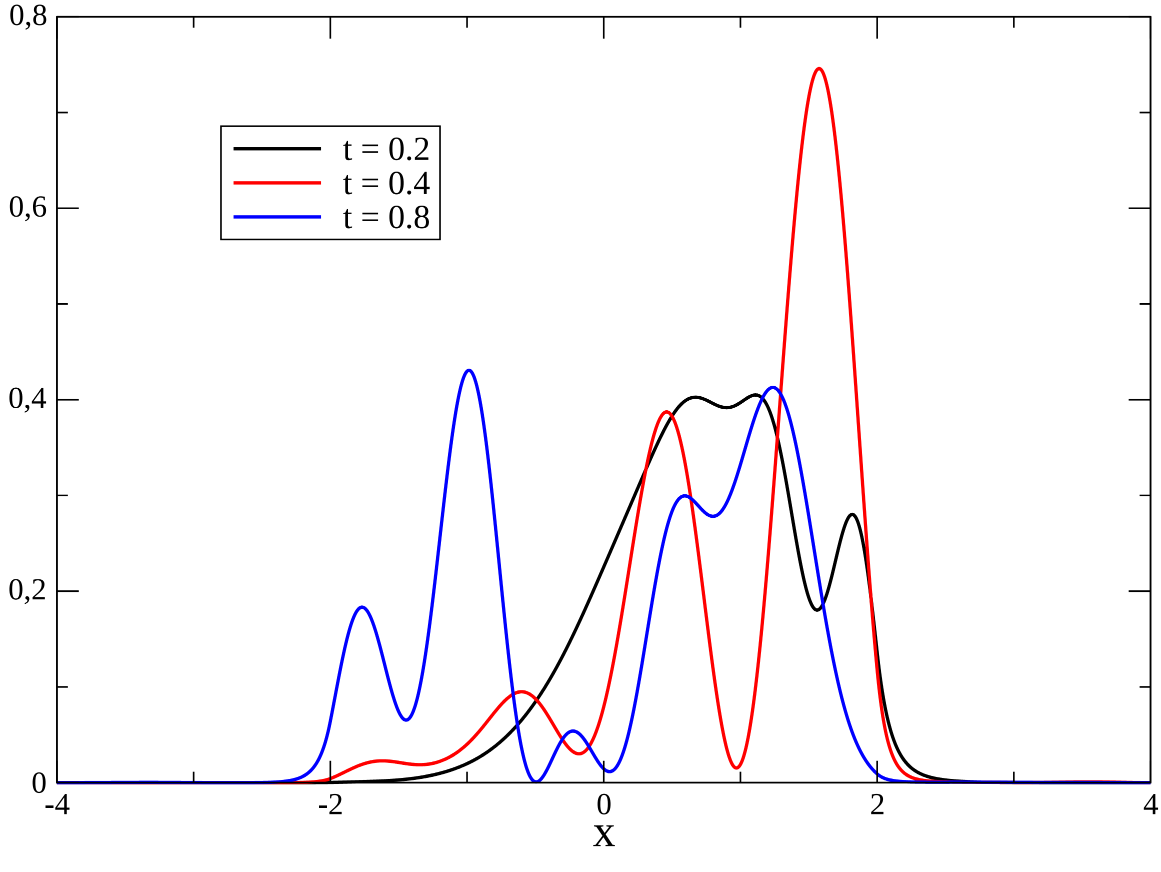
In order to damp a parasitic wave reflected from the boundary we formulate near the boundary an absorbing layer with the absorbing coefficient α. Let us consider the extended domain with $X = 3$ and take the following absorbing layer

$$\alpha(x) = \begin{cases} 0 & \text{if} \quad |x| \leq 2.5, \\ \alpha_0 & \text{otherwise.} \end{cases}$$

A plot of function $|U(x_j, 0.5)|^2$.



Plots of functions $|U(x_j, t^n)|^2$, $V = 50$.



Plots of functions $|U(x_j, t^n)|^2$, $V = -50$.