Exact Absorbing Boundary Conditions for the Schrödinger Equation with Periodic Potentials at Infinity

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Time-d problem reads:

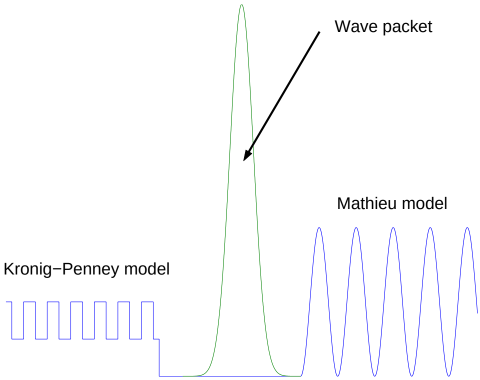
$$iu_t + u_{xx} = V(x)u,$$
$$u(x,0) = u_0(x).$$

$V(x)$: periodic at infinity;
$u_0(x)$: locally supported.

Bound state problem:

$$-u_{xx} + V(x)u = Eu,$$

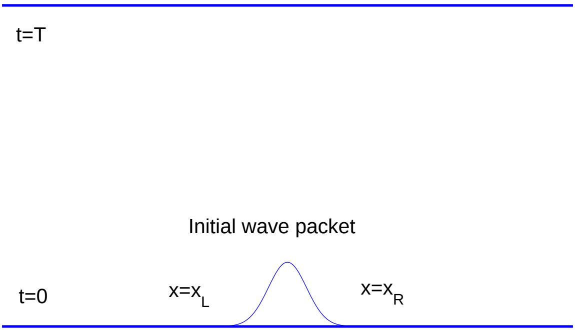
E: real energy;
u: real L^2 wave function.



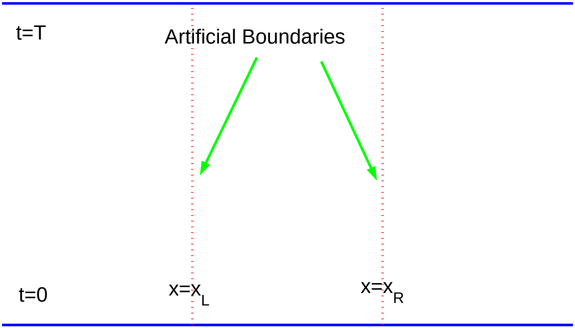
t=T

Whole definition domain

t=0


t=T
Initial wave packet
t=0
x=x_L
x=x_R

Limit the computational domain by artificial boundaries!



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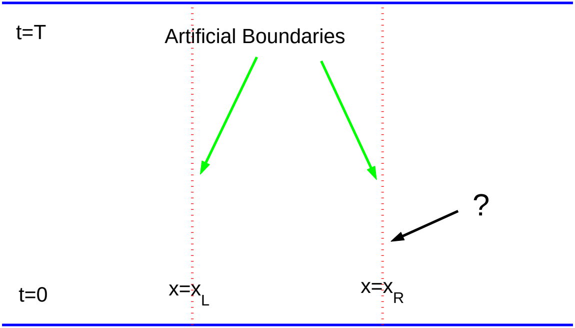

Key point: how to design the absorbing boundary condition?

Performing the Laplace transformation on

$$iu_t + u_{xx} = V(x)u, \ x > 0$$

yields

$$-\hat{u}_{xx} + V(x)\hat{u} = z\hat{u},$$

with $z = is$. Here s is the Laplace variable.

Suppose $\hat{u}_+$ is a nontrivial L^2 solution. We need to compute

$$I(z) := \frac{\hat{u}'_+(0)}{\hat{u}_+(0)}.$$

$I(z)$: the impedance. $\hat{u}_x(0) = I(z)\hat{u}(0)$: exact ABC.

OUTLINE

1. PERIODIC SECOND ORDER ODE
2. COMPUTING THE BOUND STATES FOR THE SCHRÖDINGER OPERATOR
3. TIME-D LSE WITH PERIODIC POTENTIALS AT INFINITY
4. CONCLUSION

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We consider a more general problem

$$-\frac{d}{dx}\left(\frac{1}{m(x)}\frac{dy}{dx}\right)+V(x)y=\rho(x)zy,\ x>0,$$

where m, V and ρ are S-periodic, and

$$0<M_0\le m(x)\le M_1<+\infty,\ V(x)\ge V_0,\ \rho(x)\ge \rho_0>0.$$

Two questions:

1. For what value of z, the ODE has a non-trivial L^2 solution;
2. In this case, what is the impedance? Notice that $\overline{I(z)}=I(\bar{z})$.

FIRST ORDER ODE SYSTEM

By introducing $w = \frac{1}{m(x)}\frac{dy}{dx}$, the equation

$$-\frac{d}{dx}\left(\frac{1}{m(x)}\frac{dy}{dx}\right) + V(x)y = \rho(x)zy, \; x > 0,$$

is transformed into

$$\frac{d}{dx}\begin{pmatrix} w \\ y \end{pmatrix} = \begin{pmatrix} 0 & V - \rho z \\ m & 0 \end{pmatrix}\begin{pmatrix} w \\ y \end{pmatrix}.$$

Given any vector $(w_1, y_1)^T$ at x_1, a unique $(w_2, y_2)^T$ at x_2.
Transformation matrix: $T(x, y) \in \mathcal{C}^{2\times 2}$.

$$T(x, x) = I, \; \det T(x_1, x_2) = 1,$$
$$T(x_2, x_3)T(x_1, x_2) = T(x_1, x_3),$$
$$T(x_1 + S, x_2 + S) = T(x_1, x_2).$$

Notice that

$$\frac{\partial}{\partial x} T(x_1, x) = \begin{pmatrix} 0 & V(x) - \rho(x) z \\ m(x) & 0 \end{pmatrix} T(x_1, x).$$

But

$$T(x_1, x_2) \neq e^{\int_{x_1}^{x_2} \begin{pmatrix} 0 & V(x) - \rho(x) z \\ m(x) & 0 \end{pmatrix} dx}$$

except when $m \equiv m_0$, $V \equiv V_0$ and $\rho = \rho_0$. In this case

$$T(x_1, x_2) = e^{(x_2 - x_1) \begin{pmatrix} 0 & V_0 - \rho_0 z \\ m_0 & 0 \end{pmatrix}}.$$

Floquet solution

Consider $T(0,S)$. It has two eigenvalues $e^{\pm\mu S}$ with $\Re\mu \leq 0$ since $\det T(x,y) = 1$. If $\Re\mu < 0$, then two eigenvalues are distinct. Suppose $(c_\pm, d_\pm)^T$ are the associated eigenvectors.

$$T(0,x)(c_\pm, d_\pm)^T$$

are two linearly independent solutions. Besides,

$$e^{\mp\mu x} T(0,x)(c_\pm, d_\pm)^T$$

are periodic functions. Thus

$$T(0,x)(c_+, d_+)^T = e^{\mu x} e^{-\mu x} T(0,x)(c_+, d_+)^T$$

is an L^2 solution. L^2 solution $\leftrightarrow \Re\mu < 0 \leftrightarrow |e^{\mu S}| < 1$.

$$I(z) = \frac{y'(0)}{y(0)} = m(0)\frac{c_+}{d_+}.$$

EXAMPLE: $m(x) = m_0$, $V(x) = V_0$ AND $\rho(x) = \rho_0$

In this case,

$$T(0,S) = e^{S\begin{pmatrix} 0 & V_0 - \rho_0 z \\ m_0 & 0 \end{pmatrix}}.$$

is constant. The eigenvalues are $e^{\pm\mu S}$ with

$$\mu = -\sqrt[+]{m_0(V_0 - \rho_0 z)} \quad \text{if} \quad \Im z \neq 0 \text{ or } \Re z < \frac{V_0}{\rho_0}.$$

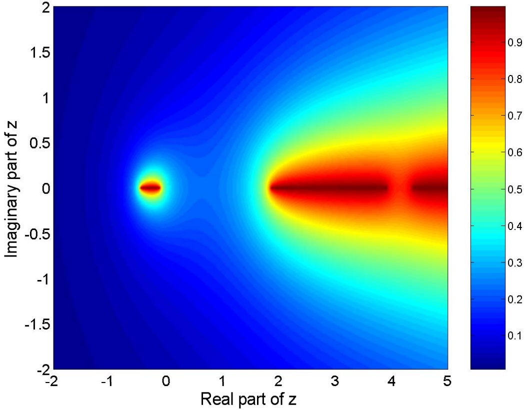
The eigenvector associated with $e^{\mu S}$ is

$$(c_+, d_+) = (\mu, m_0)^T.$$

Thus

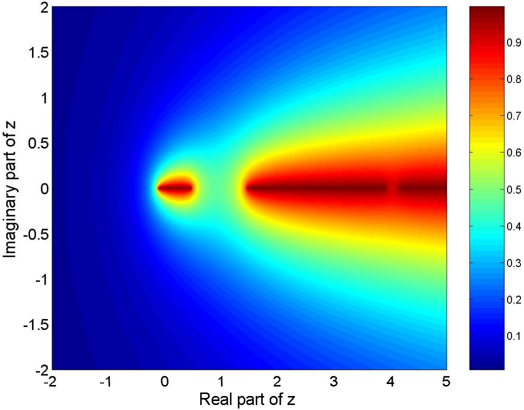
$$I(z) = \mu = -\sqrt[+]{m_0\rho_0}\sqrt[+]{\frac{V_0}{\rho_0} - z}.$$

EXAMPLE: $m(x) = \rho(x) = 1$ AND $V(x) = 2\cos(2x)$



Modulus of $e^{\mu S}$ with respect to z.

EXAMPLE: $m(x) = \rho(x) = 1 + \cos(2x)/5$ AND $V(x) = \sin(2x)$



Modulus part of $e^{\mu S}$ with respect to z.

Stop bands

It turns out that those ending points of real intervals are nothing but the eigenvalues of the periodic characteristic problem:

Find $\lambda \in \mathbf{R}$ and $y \in C^1_{per}[0, 2S]$, such that

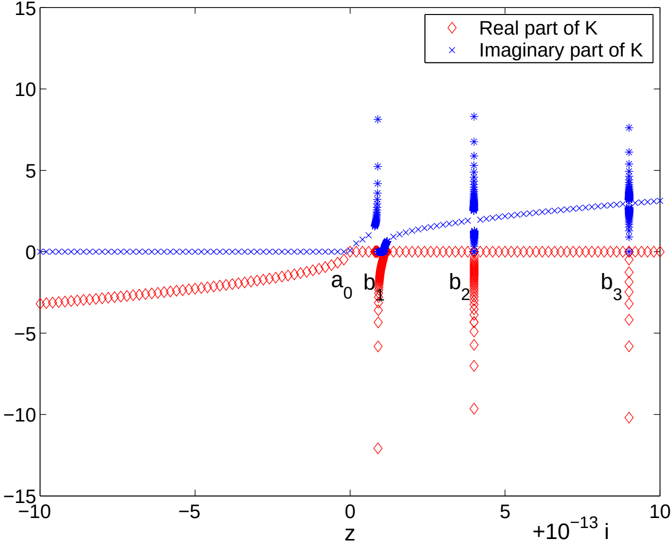
$$-\frac{d}{dx}\left(\frac{1}{m(x)}\frac{dy}{dx}\right) + V(x)y = \rho(x)\lambda y.$$

Those real points at which the Floquet's factor has a modulus less than 1 constitute a series of intervals

$$(-\infty, x_1),\ (x_2, x_3),\ \cdots$$

They are called stop bands.
Conclusion: for all z with $\Im z \neq 0$ or in the stop bands, periodic 2nd ODE has a nontrivial L^2 solution.

EXAMPLE: $V(x) = 0.2\cos(2x)$, $m = \rho = 1$



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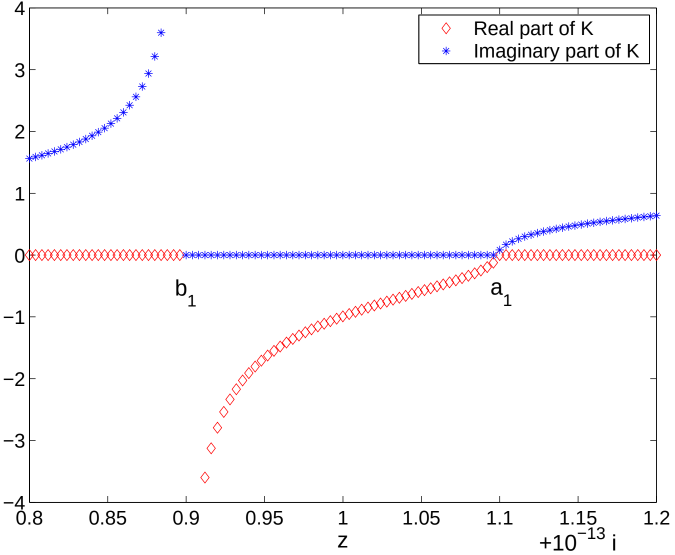

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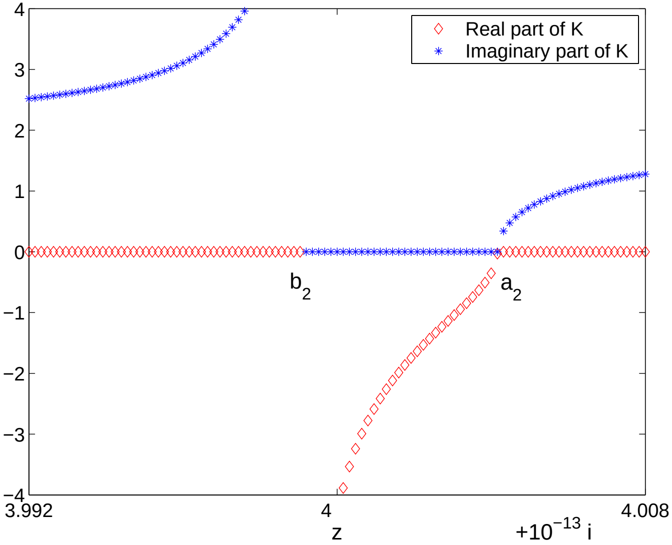

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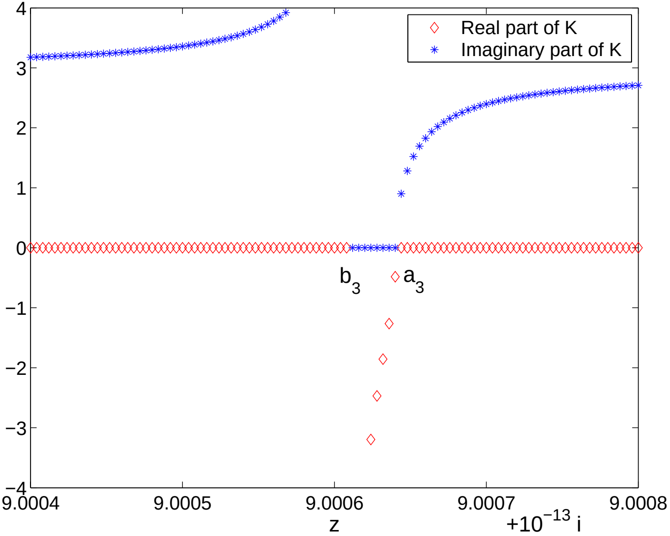


A careful observation reveals that

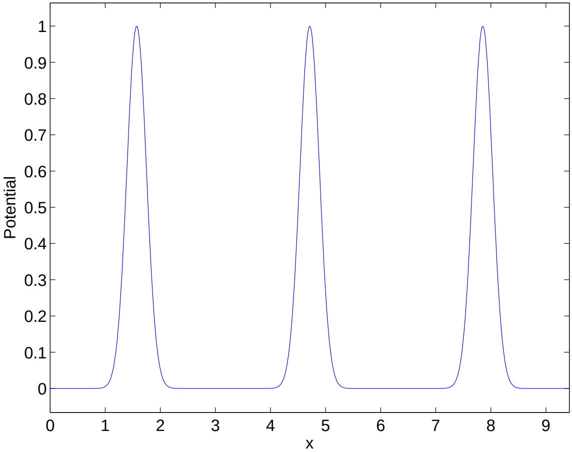
- Both turning points a_i and singular points b_i are eigenvalues of the characteristic problem;
- a_i is associated with an even eigenfunction;
- b_i is associated with an odd eigenfunction;
- The singularity behaves like $1/\sqrt[+]{b_i - z}$;
- The solution around turning points behaves like $\sqrt[+]{a_i - z}$.

We conjecture that

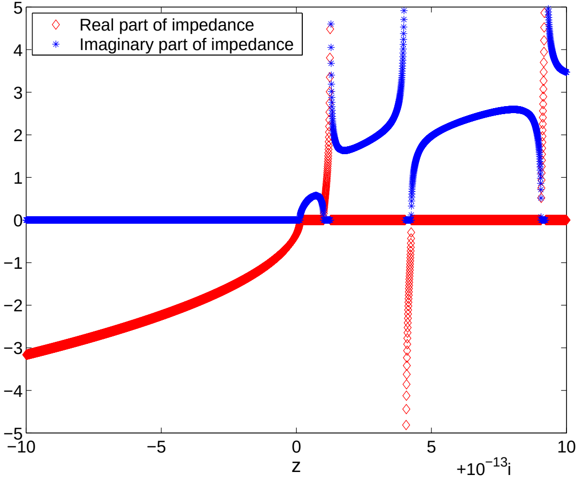
$$I(z) = -\sqrt{m(0)\rho(0)}\,\sqrt[+]{-z + a_0}\prod_{r=1}^{+\infty}\frac{\sqrt[+]{-z + a_r}}{\sqrt[+]{-z + b_r}}.$$

for all symmetric m, V and ρ.

Example: periodic Gaussian $V = \sum_{n=-\infty}^{+\infty} e^{-16(x-\pi/2-n\pi)^2}$, $m = \rho = 1$

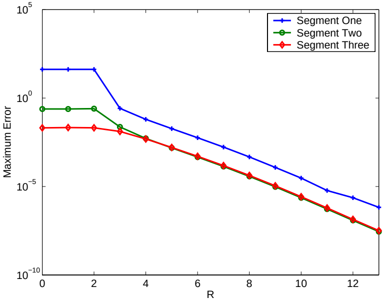


Example: periodic Gaussian pulse $V = \sum_{n=-\infty}^{+\infty} e^{-16(x-\pi/2-n\pi)^2}$, $m = \rho = 1$



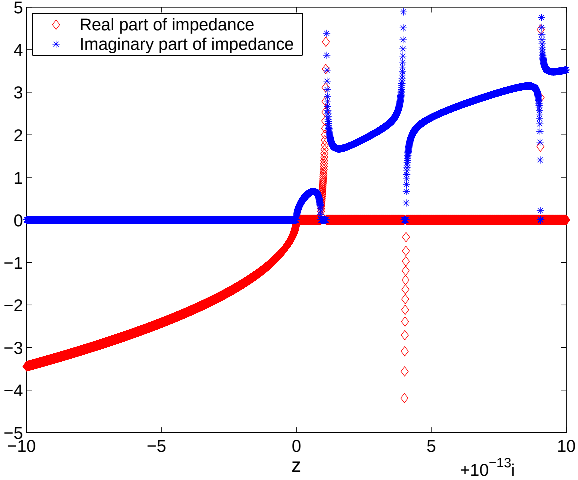
EXAMPLE: PERIODIC GAUSSIAN PULSE $V = \sum_{n=-\infty}^{+\infty} e^{-16(x-\pi/2-n\pi)^2}$, $m = \rho = 1$

$$I_R(z) = -\sqrt{m(0)\rho(0)}\,\sqrt[+]{-z+a_0}\prod_{r=1}^{R}\frac{\sqrt[+]{-z+a_r}}{\sqrt[+]{-z+b_r}}.$$



Seg. One: $[-10, 10] + 10^{-13}i$. Seg. Two: $[-10, 10] + i$. Seg. Three: $[-10, 10] + 10i$.

EXAMPLE: $V = 0$, $m = 1$, $\rho = 1 + \cos(2x)/5$



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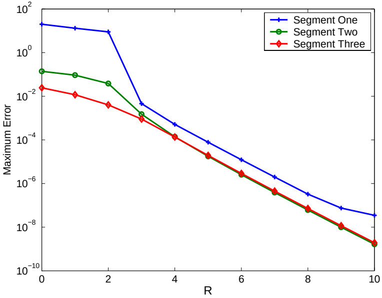

Seg. One: $[-10, 10] + 10^{-13}i$. Seg. Two: $[-10, 10] + i$. Seg. Three: $[-10, 10] + 10i$.

Numerical evidences have already shown that

$$I(z) = -\sqrt{m(0)\rho(0)}\sqrt[+]{-z+a_0}\prod_{r=1}^{+\infty}\frac{\sqrt[+]{-z+a_r}}{\sqrt[+]{-z+b_r}}.$$

when $\Im z \neq 0$. This result can be further generalized for those real z in the stop bands. In this case

$$I(z) = \lim_{\text{real } \epsilon\to 0} I(z \pm \epsilon).$$

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Computing the bound states for the Schrödinger operator

Suppose

$$V(x) = \begin{cases} V_{per}^L, & x < x_L, \\ V_{int}, & x_L < x < x_R, \\ V_{per}^R, & x > x_R. \end{cases}$$

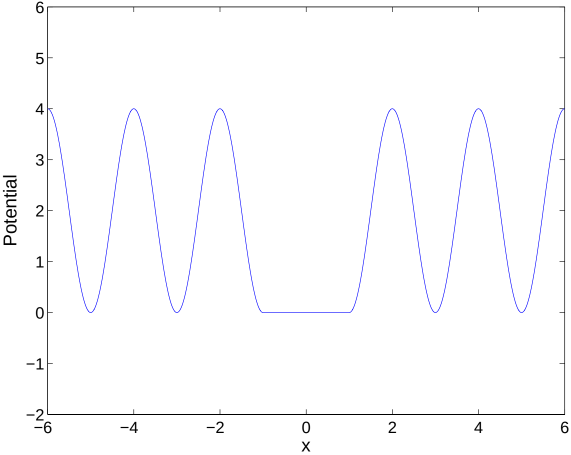
V_{per}^L and V_{per}^R are periodic. Given E, we solve

$$\begin{aligned} &-u_{xx} + V(x)u = \Phi(E)u, \ x_L < x < x_R, \\ &-u_x = I_L(E)u, \ x = x_L, \\ &u_x = I_R(E)u, \ x = x_R. \end{aligned}$$

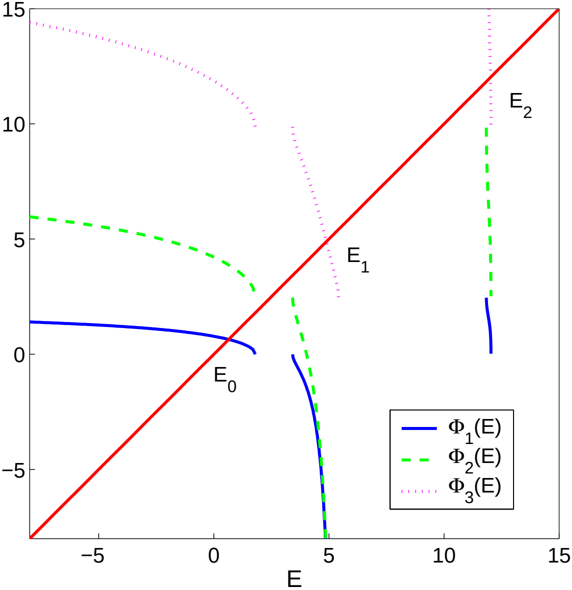
E lies in one of the stop bands. The energy associated with bound state satisfies $E = \Phi(E)$. Algorithm: Newton-Steffenson iterations

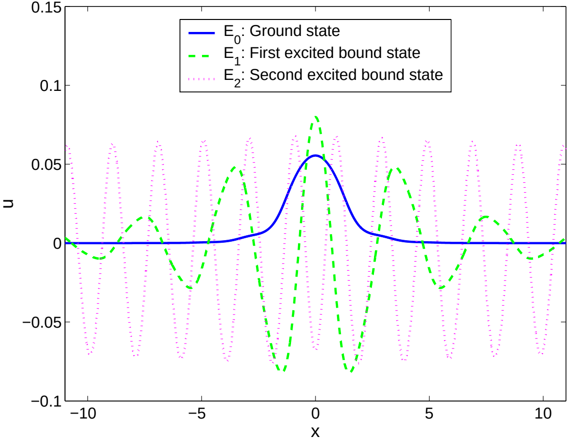
Consider

$$V(x) = \begin{cases} 2 + 2\cos(\pi x), & |x| > 1, \\ 0, & |x| < 1. \end{cases}$$



AN EXAMPLE





$E_0 = 6.42647(-1)$. $E_1 = 4.88649$. $E_2 = 1.20164(1)$.

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The equation reads

$$iu_t + u_{xx} = V(x)u.$$

We have $z = is$. The right ABC reads

$$\hat{u}_x(x_R, s) = -\sqrt[+]{-is + a_0} \prod_{r=1}^{+\infty} \frac{\sqrt[+]{-is + a_r}}{\sqrt[+]{-is + b_r}} \hat{u}(x_R, s), \ \Re s > 0.$$

Introduce a sequence of auxiliary functions

$$\hat{w}_k(s) \overset{def}{=} \prod_{r=k}^{+\infty} \frac{\sqrt[+]{-is + a_r}}{\sqrt[+]{-is + b_r}} \hat{u}(x_R, s), \ k = 1, 2, \cdots ,$$

Then the exact ABC is rewritten as

$$\hat{u}_x(x_R, s) + \sqrt[+]{-is + a_0}\, \hat{w}_1(s) = 0,$$
$$\sqrt[+]{-is + b_k}\, \hat{w}_k = \sqrt[+]{-is + a_k}\, \hat{w}_{k+1}, \ k = 1, 2, \cdots .$$

In the physical space, it becomes

$$u_x(x_R,t) + e^{-i\pi/4} e^{-ia_0 t} \partial_t^{\frac{1}{2}} \left(e^{ia_0 t} w_1(t) \right) = 0,$$

$$e^{-ib_k t} \partial_t^{\frac{1}{2}} (e^{ib_k t} w_k) = e^{-ia_k t} \partial_t^{\frac{1}{2}} (e^{ia_k t} w_{k+1}),\ k = 1, 2, \cdots .$$

Two questions:

- The sequence of w_k should be truncated;
- $\partial_t^{\frac{1}{2}}$ should be evaluated efficiently.

The potential is

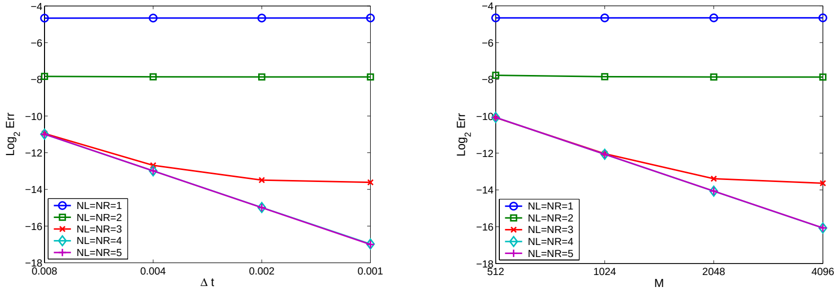
$$V = 2\cos(2x),\ x \in \mathbf{R},$$

and the initial function is

$$u_0(x) = e^{-x^2+2ix}.$$

The computational domain is $[-2\pi, 2\pi]$.
Algorithm: Crank-Nicolson+2nd central difference+2nd discretization of $\partial_t^{\frac{1}{2}}$+Fast evaluation

Accuracy test



Here, *NL* and *NR* stand for the numbers of auxiliary functions at the left and right boundary points, respectively.

Interaction of a wave packet with periodic potentials

The potential is set as

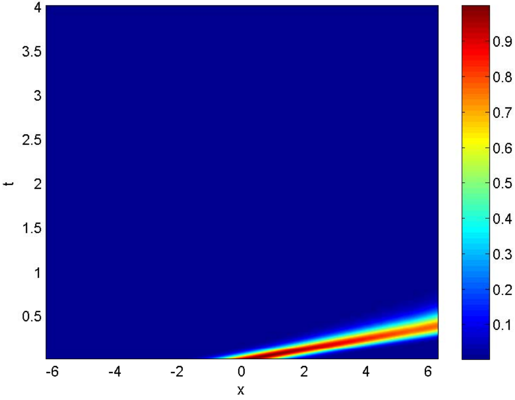
$$V(x) = \begin{cases} 2q_L \cos \frac{2\pi(x+2\pi)}{S_L}, & x \in \left(-\infty, -2\pi + \frac{S_L}{4}\right), \\ 0, & x \in \left(-2\pi + \frac{S_L}{4}, 2\pi - \frac{S_R}{4}\right), \\ 2q_R \cos \frac{2\pi(x-2\pi)}{S_R}, & x \in \left(2\pi - \frac{S_R}{4}, +\infty\right). \end{cases}$$

The initial function is

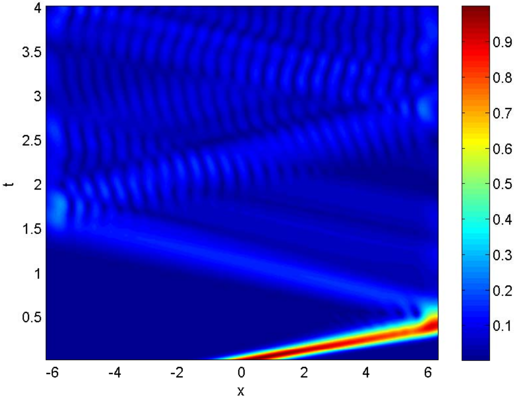
$$u_0(x) = e^{-x^2+8ix}.$$

CASE A

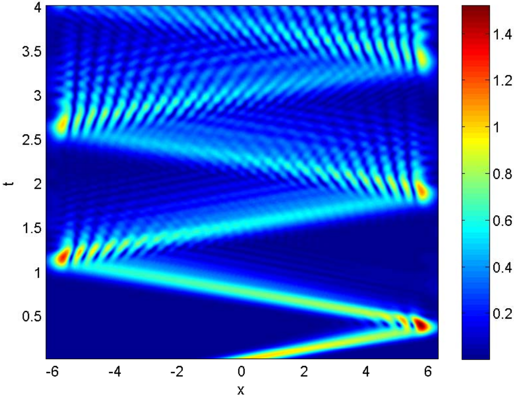
$$S_L = S_R = \pi, \; q_L = q_R = 5.$$



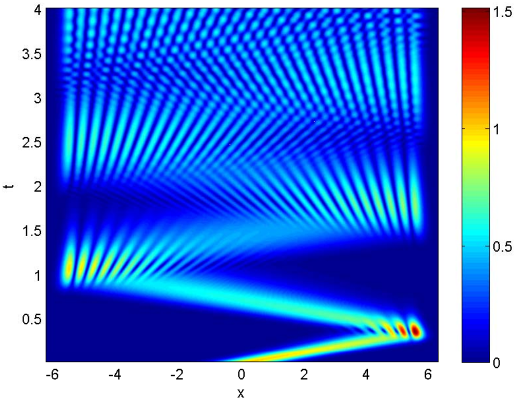
$$S_L = S_R = \pi, \; q_L = q_R = 20.$$



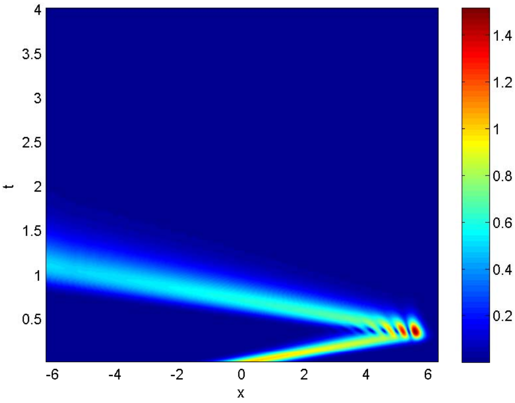
$$S_L = S_R = \pi, \ q_L = q_R = 50.$$



$$S_L = S_R = \pi, \; q_L = q_R = 100.$$

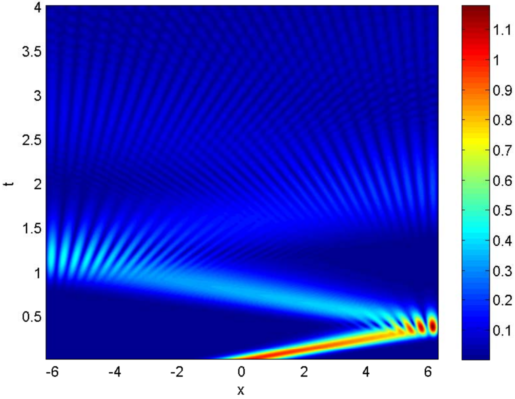


$$S_L = S_R = \pi,\ q_L = 5,\ q_R = 100.$$

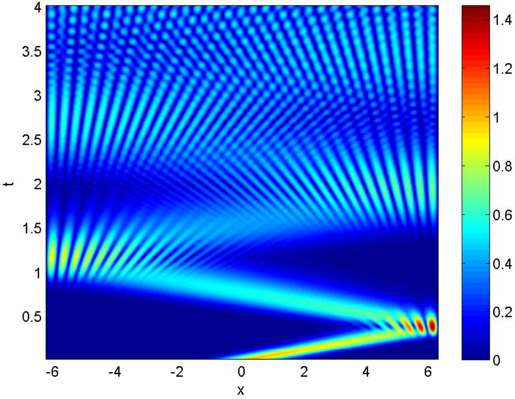


CASE F

$$S_L = S_R = \frac{\pi}{20}, \; q_L = q_R = 200.$$



$$S_L = S_R = \frac{\pi}{20}, \; q_L = q_R = 1000.$$



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Conclusion

- Periodic second order ODE problem has been studied;
- The impedance is explicitly given when the coefficients are symmetric;
- A method for computing bound states of the Schrödinger operator has been proposed;
- Exact ABC for the time-d Schrödinger equation with periodic potentials has been presented and implemented;
- Currently under working: more general periodic structure problems;
- Unsolved task: prove the proposed conjecture theoretically;
- More challenging: high-dimensional periodic structure problems.