COMM. MATH. SCI.
Vol. 2, No. 1, pp. 79–94

EXACT ARTIFICIAL BOUNDARY CONDITIONS FOR THE SCHRÖDINGER EQUATION IN $\mathbb{R}^2$ *

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Abstract. In this paper, we propose a class of exact artificial boundary conditions for the numerical solution of the Schrödinger equation on unbounded domains in two-dimensional cases. After we introduce a circular artificial boundary, we get an initial-boundary problem on a disc enclosed by the artificial boundary which is equivalent to the original problem. Based on the Fourier series expansion and the special functions techniques, we get the exact artificial boundary condition and a series of approximating artificial boundary conditions. When the potential function is independent of the radiant angle θ, the problem can be reduced to a series of one-dimensional problems. That can reduce the computational complexity greatly. Our numerical examples show that our method gives quite good numerical solutions with no numerical reflections.

Key words. Schrödinger Equation, Unbounded domain, Artificial boundary condition.

1. Introduction

The Schrödinger type equation is one of the most important models of mathematical physics, with applications to different fields such as quantum mechanics, nonlinear optics, plasma physics, and so on. Many such physical problems are described in unbounded domains. Therefore, lots of mathematicians and engineers are devoted to the study of the non-reflecting boundary conditions for Schrödinger equation in unbounded domains. Some of them have derived so-called *transparent boundary conditions* (TBCs) or *absorbing boundary conditions* (ABCs) [1, 2, 3, 4, 7, 8, 11, 13]. In these papers, first they take a Fourier (or Laplace) transformation in time, then get a Helmholtz equation; using the expression of solution by Hankel functions, they get the ABCs in Fourier space; after making an approximation of the global integrals and an inverse Fourier transformation, they get the ABCs for the original problem. Here, they need to deal with the integrals with strong singularity very carefully [3]. Other people have given the *perfectly matching layers* method for these problems [6, 12]. We want to give an exact, flexible and convenient artificial boundary condition for this problem in two dimensional cases.

Here we consider the following Schrödinger Equation in $\mathbb{R}^2$:

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\triangle\psi + V(x,t)\psi, \quad x\in\mathbb{R}^2,\ 0<t\le T, \tag{1.1}$$
$$\psi|_{t=0} = \psi^0(x), \quad x\in\mathbb{R}^2, \tag{1.2}$$
$$\psi \longrightarrow 0, \text{ when } |x|\longrightarrow +\infty,\ 0<t\le T. \tag{1.3}$$

where $V(x,t)$ is the given potential function and $\psi^0(x)$ is the given initial data.

We suppose that the potential function $V(x,t)$ is a constant outside of a disc

*Received: September 3, 2003; accepted (in revised version): December 23, 2003. Communicated by Shi Jin.

This work was supported by the Special Funds for Major State Basic Research Projects of China. The second author was also supported by NSFC under the Project 10301017 and the Basic Research Projects of Tsinghua University.

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$\Omega_R = \{x \bigm| |x| < R\}$, namely:

$$V(x,t) = V_\infty, \text{ when } |x| \geq R. \tag{1.4}$$

Moreover, we assume that the initial function $\psi^0(x)$ is compactly supported and

$$supp\{\psi^0(x)\} \subset \Omega_R.$$

We introduce an artificial boundary in $\mathbb{R}^2$:

$$\Gamma_R = \left\{x \bigm| |x| = R\right\}, \tag{1.5}$$

Γ_R divides $\mathbb{R}^2$ into two parts, the bounded part $\Omega_R = \{x \bigm| |x| < R\}$ and the unbounded part $\Omega_e = \{x \bigm| |x| > R\}$. Then the problem (1.1)–(1.3) can be rewritten in the coupled form:

$$\begin{aligned}
i\frac{\partial\psi}{\partial t} &= -\frac{1}{2}\triangle\psi + V(x,t)\psi, \quad x \in \Omega_R,\ 0 < t \leq T, && (1.6)\\
\psi|_{t=0} &= \psi^0(x), \quad x \in \Omega_R, && (1.7)\\
i\frac{\partial\psi}{\partial t} &= -\frac{1}{2}\triangle\psi + V(x,t)\psi, \quad x \in \Omega_e,\ 0 < t \leq T, && (1.8)\\
\psi|_{t=0} &= 0, \quad x \in \Omega_e, && (1.9)\\
\psi &\longrightarrow 0, \text{ when } |x| \longrightarrow +\infty,\ 0 < t \leq T. && (1.10)
\end{aligned}$$

Moreover

$$\psi(x,t) \text{ and } \frac{\partial\psi}{\partial r} \text{ are continuous on the artificial boundary } \Gamma_R \times [0,T]. \tag{1.11}$$

The problem (1.6)–(1.11) is a coupled problem, the problem (1.6)–(1.7) or problem (1.8)–(1.10) can not be solved independently without the connecting condition (1.11). The main goal of this paper is to derive the artificial boundary condition for Schrödinger equation on the artificial boundary $\Gamma_R \times [0,T]$.

2. The exact artificial boundary condition on the artificial boundary $\Gamma_R \times [0,T]$

Suppose that $\psi(x,t)$ is the solution of problem (1.1)–(1.3), the restriction of $\psi(x,t)$ on $\Omega_e \times (0,T]$ satisfies problem (1.8)–(1.10). If the value $\psi|_{|x|=R}$ is given, namely

$$\psi|_{|x|=R} = \psi(R,\theta,t), \tag{2.1}$$

then the problem (1.8)–(1.10) and (2.1) is well posed. For the solution in the polar coordinates, $\psi(r,\theta,t)$, of the problem (1.8)–(1.10) and (2.1), we have the Fourier expansion:

$$\psi(r,\theta,t) = \frac{\psi_0(r,t)}{2} + \sum_{n=1}^{\infty}(\psi_n(r,t)\cos n\theta + \phi_n(r,t)\sin n\theta), \tag{2.2}$$

with

$$\psi_n(r,t) = \frac{1}{\pi}\int_0^{2\pi}\psi(r,\theta,t)\cos n\theta\, d\theta,\ n = 0,1,\cdots \tag{2.3}$$

$$\phi_n(r,t) = \frac{1}{\pi}\int_0^{2\pi}\phi(r,\theta,t)\sin n\theta\, d\theta,\ n = 1,2,\cdots \tag{2.4}$$

and

$$\psi(R,\theta,t) = \frac{\psi_0(R,t)}{2} + \sum_{n=1}^{\infty}(\psi_n(R,t)\cos n\theta + \phi_n(R,t)\sin n\theta). \tag{2.5}$$

Substituting (2.2) and (2.5) into the problem (1.8)–(1.10) and (2.1), for $\psi_n(r,t)$ $(n = 0, 1, 2, \cdots)$ and $\phi_n(r,t)(n = 1, 2, \cdots)$ we obtain:

$$\begin{aligned}
i\frac{\partial\psi_n}{\partial t} &= -\frac{1}{2}(\frac{\partial^2\psi_n}{\partial r^2} + \frac{1}{r}\frac{\partial\psi_n}{\partial r} - \frac{n^2}{r^2}\psi_n) + V_\infty\psi_n, \quad R < r < +\infty,\ 0 < t \le T, & (2.6)\\
\psi_n|_{r=R} &= \psi_n(R,t), \quad 0 < t \le T, & (2.7)\\
\psi_n|_{t=0} &= 0, \quad R \le r < +\infty, & (2.8)\\
\psi_n &\longrightarrow 0, \quad \text{when} \quad r \longrightarrow +\infty,\ 0 < t \le T. & (2.9)
\end{aligned}$$

$$\begin{aligned}
i\frac{\partial\phi_n}{\partial t} &= -\frac{1}{2}(\frac{\partial^2\phi_n}{\partial r^2} + \frac{1}{r}\frac{\partial\phi_n}{\partial r} - \frac{n^2}{r^2}\phi_n) + V_\infty\phi_n, \quad R < r < +\infty,\ 0 < t \le T, & (2.10)\\
\phi_n|_{r=R} &= \phi_n(R,t), \quad 0 < t \le T, & (2.11)\\
\phi_n|_{t=0} &= 0, \quad R \le r < +\infty, & (2.12)\\
\phi_n &\longrightarrow 0, \quad \text{when} \quad r \longrightarrow +\infty,\ 0 < t \le T. & (2.13)
\end{aligned}$$

For $n = 0, 1, \cdots$, we discuss the solution $\psi_n(r,t)$ of problem (2.6)–(2.9). Let

$$\psi_n(r,t) = w_n(r,t)\ e^{-iV_\infty t}, \tag{2.14}$$

then $w_n(r,t)$ satisfies:

$$\begin{aligned}
i\frac{\partial w_n}{\partial t} &= -\frac{1}{2}(\frac{\partial^2 w_n}{\partial r^2} + \frac{1}{r}\frac{\partial w_n}{\partial r} - \frac{n^2}{r^2}w_n), \quad R < r < +\infty,\ 0 < t \le T, & (2.15)\\
w_n|_{r=R} &= \psi_n(R,t)e^{iV_\infty t} \ \equiv\ w_n(R,t), \quad 0 < t \le T, & (2.16)\\
w_n|_{t=0} &= 0, \quad R \le r < +\infty, & (2.17)\\
w_n &\longrightarrow 0, \quad \text{when} \quad r \longrightarrow +\infty, \quad 0 < t \le T. & (2.18)
\end{aligned}$$

We now solve the problem (2.15)–(2.18) for given $w_n(R,t)$ using the approach given in [10]. First we consider the following simplified problem:

$$\begin{aligned}
i\frac{\partial G_n}{\partial t} &= -\frac{1}{2}(\frac{\partial^2 G_n}{\partial r^2} + \frac{1}{r}\frac{\partial G_n}{\partial r} - \frac{n^2}{r^2}G_n), \quad R < r < +\infty, 0 < t \le T, & (2.19)\\
G_n|_{r=R} &= 1, \quad 0 < t \le T, & (2.20)\\
G_n|_{t=0} &= 0, \quad R \le r < +\infty, & (2.21)\\
G_n &\longrightarrow 0, \quad \text{when} \quad r \longrightarrow +\infty,\ 0 < t \le T. & (2.22)
\end{aligned}$$

For any $\mu > 0$, let

$$G_n(r,t) = U(r)e^{-\frac{i}{2}\mu^2 t}. \tag{2.23}$$

Substituting (2.23) into (2.19), we obtain that $U(r)$ satisfies:

$$\frac{\partial^2 U}{\partial r^2} + \frac{1}{r}\frac{\partial U}{\partial r} + \left(\mu^2 - \frac{n^2}{r^2}\right)U = 0. \tag{2.24}$$

Equation (2.24) is the Bessel equation of order n, and $J_n(\mu r), Y_n(\mu r)$ are two independent solutions of it. Hence

$$e^{-\frac{i}{2}\mu^2 t}\frac{J_n(\mu r)Y_n(\mu R) - Y_n(\mu r)J_n(\mu R)}{J_n^2(\mu R) + Y_n^2(\mu R)}$$

is a solution of equation (2.24) for any $\mu > 0$. Let

$$G_*(r,t) = \frac{2}{\pi}\int_0^{+\infty} e^{-\frac{i}{2}\mu^2 t}\frac{J_n(\mu r)Y_n(\mu R) - Y_n(\mu r)J_n(\mu R)}{J_n^2(\mu R) + Y_n^2(\mu R)}\frac{d\mu}{\mu}. \tag{2.25}$$

$G_*(r,t)$ is a solution of equation (2.24) and

$$\begin{aligned} G_*(r,t)|_{r=R} &= 0, \\ G_*(r,t)|_{t=0} &= \frac{2}{\pi}\int_0^{+\infty} \frac{J_n(\mu r)Y_n(\mu R) - Y_n(\mu r)J_n(\mu R)}{J_n^2(\mu R) + Y_n^2(\mu R)}\frac{d\mu}{\mu} \\ &= -\left(\frac{R}{r}\right)^n, \quad r > R. \end{aligned}$$

The last equality is given in [9] (pp. 665). Let

$$G_n(r,t) = \left(\frac{R}{r}\right)^n + G_*(r,t). \tag{2.26}$$

It is straightforward to check that $G_n(r,t)$ is the solution of problem (2.19)–(2.22). By Duhamel's theorem and the solution $G_n(r,t)$, we obtain $w_n(r,t)$, the solution of problem (2.15)–(2.18):

$$\begin{aligned} w_n(r,t) &= \int_0^t w_n(R,\lambda)\frac{\partial G_n(r,t-\lambda)}{\partial t}d\lambda \\ &= -\int_0^t w_n(R,\lambda)\frac{\partial G_n(r,t-\lambda)}{\partial \lambda}d\lambda \\ &= -\{w_n(R,\lambda)G_n(r,t-\lambda)\}\Big|_{\lambda=0}^{\lambda=t} + \int_0^t \frac{\partial w_n(R,\lambda)}{\partial \lambda}G_n(r,t-\lambda)d\lambda \\ &= \int_0^t \frac{\partial w_n(R,\lambda)}{\partial \lambda}G_n(r,t-\lambda)d\lambda. \end{aligned}$$

By the transformation (2.14), we obtain $\psi_n(r,t), (n = 0, 1, \cdots)$, the solution of problem (2.6)–(2.9), and $\phi_n(r,t), (n = 1, 2, \cdots)$, the solution of problem (2.10)–(2.13). Namely

$$\psi_n(r,t) = e^{-iV_\infty t}\int_0^t \frac{\partial}{\partial \lambda}(\psi_n(R,\lambda)e^{iV_\infty \lambda})G_n(r,t-\lambda)d\lambda, \quad \text{for } n = 0, 1, \cdots$$

$$\phi_n(r,t) = e^{-iV_\infty t}\int_0^t \frac{\partial}{\partial \lambda}(\phi_n(R,\lambda)e^{iV_\infty \lambda})G_n(r,t-\lambda)d\lambda, \quad \text{for } n = 1, 2, \cdots$$

Furthermore,

$$\frac{\partial \psi_n}{\partial r}\Big|_{r=R} = \int_0^t \frac{\partial}{\partial \lambda}(\psi_n(R,\lambda)e^{iV_\infty(\lambda - t)})\frac{\partial G_n}{\partial r}(R,t-\lambda)d\lambda, \quad \text{for } n = 0, 1, \cdots \tag{2.27}$$

$$\frac{\partial \phi_n}{\partial r}\Big|_{r=R} = \int_0^t \frac{\partial}{\partial \lambda}(\phi_n(R,\lambda)e^{iV_\infty(\lambda - t)})\frac{\partial G_n}{\partial r}(R,t-\lambda)d\lambda, \quad \text{for } n = 1, 2, \cdots \tag{2.28}$$

On the other hand,

$$\frac{\partial G_n}{\partial r}(r,t)\Big|_{r=R} = -\frac{n}{R} + \frac{2}{\pi}\int_0^{+\infty} e^{-\frac{i}{2}\mu^2 t}\frac{J_n'(\mu R)Y_n(\mu R) - Y_n'(\mu R)J_n(\mu R)}{J_n^2(\mu R)+Y_n^2(\mu R)}d\mu$$
$$= -\frac{n}{R} - \frac{4}{\pi^2 R}\int_0^{+\infty}\frac{e^{-\frac{i}{2}\mu^2 t}}{J_n^2(\mu R)+Y_n^2(\mu R)}\frac{d\mu}{\mu}.$$

The last equality is from the Wronskian relation

$$J_n'(\mu R)Y_n(\mu R) - Y_n'(\mu R)J_n(\mu R) = -\frac{2}{\pi\mu R}.$$

Let

$$S_n(t) = \frac{4\sqrt{t}}{\sqrt{\pi^3}}\int_0^{+\infty}\frac{e^{-\frac{i}{2}\mu^2 t}}{J_n^2(\mu R)+Y_n^2(\mu R)}\frac{d\mu}{\mu}, \tag{2.29}$$

then

$$\frac{\partial G_n(r,t)}{\partial r}\Big|_{r=R} = -\frac{n}{R} - \frac{S_n(t)}{\sqrt{\pi t}}. \tag{2.30}$$

Substituting (2.30) into (2.27) and (2.28), we have:

$$\frac{\partial \psi_n}{\partial r}\Big|_{r=R} = -\frac{n}{R}\psi_n(R,t) - \frac{1}{\sqrt{\pi}}\int_0^t \frac{\partial}{\partial\lambda}\left(\psi_n(R,\lambda)e^{iV_\infty(\lambda-t)}\right)\frac{S_n(t-\lambda)}{\sqrt{t-\lambda}}d\lambda, \tag{2.31}$$
$$\frac{\partial \phi_n}{\partial r}\Big|_{r=R} = -\frac{n}{R}\phi_n(R,t) - \frac{1}{\sqrt{\pi}}\int_0^t \frac{\partial}{\partial\lambda}\left(\phi_n(R,\lambda)e^{iV_\infty(\lambda-t)}\right)\frac{S_n(t-\lambda)}{\sqrt{t-\lambda}}d\lambda. \tag{2.32}$$

Furthermore, by the expansion (2.2) we get

$$\frac{\partial \psi}{\partial r}\Big|_{r=R} = \frac{1}{2}\frac{\partial \psi_0}{\partial r}\Big|_{r=R} + \sum_{n=1}^{\infty}\left(\frac{\partial \psi_n}{\partial r}\Big|_{r=R}\cos n\theta + \frac{\partial \phi_n}{\partial r}\Big|_{r=R}\sin n\theta\right). \tag{2.33}$$

Substituting (2.31), (2.32) into (2.33), and using (2.5), we have

$$\begin{aligned}\frac{\partial \psi}{\partial r}\Big|_{r=R} = &-\frac{1}{2\sqrt{\pi^3}}\int_0^t\int_0^{2\pi}\frac{\partial}{\partial\lambda}\left(\psi(R,\xi,\lambda)e^{iV_\infty(\lambda-t)}\right)\frac{S_0(t-\lambda)}{\sqrt{t-\lambda}}d\xi d\lambda\\ &-\sum_{n=1}^{\infty}\left\{\frac{n}{R\pi}\int_0^{2\pi}\psi(R,\xi,t)\cos n(\xi-\theta)d\xi\right.\\ &\left.+\frac{1}{\sqrt{\pi^3}}\int_0^t\int_0^{2\pi}\frac{\partial}{\partial\lambda}\Big(\psi(R,\xi,\lambda)\cos n(\theta-\xi)e^{iV_\infty(\lambda-t)}\Big)\frac{S_n(t-\lambda)}{\sqrt{t-\lambda}}d\xi d\lambda\right\}\\ \equiv{}& \Lambda_\infty\big(\psi|_{|x|=R},\theta,t\big).\end{aligned} \tag{2.34}$$

This is the exact boundary condition satisfied by the solution of problem (1.1)–(1.3). Therefore, the problem (1.1)–(1.3) is equivalent to the following boundary value problem on the bounded domain $\Omega_R\times[0,T]$:

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\triangle\psi + V(x,t)\psi, \quad x\in\Omega_R,\ 0<t\le T, \tag{2.35}$$
$$\psi\big|_{t=0} = \psi^0(x), \quad x\in\Omega_R, \tag{2.36}$$
$$\frac{\partial\psi}{\partial r}\Big|_{|x|=R} = \Lambda_\infty\big(\psi|_{|x|=R},\theta,t\big), \quad 0<t\le T. \tag{2.37}$$

In practice, we need to truncate the series in (2.37),

$$\frac{\partial\psi}{\partial r}\Big|_{|x|=R} = \Lambda_N\big(\psi|_{|x|=R}, \theta, t\big), \tag{2.38}$$

that means we only use the summation of first $N+1$ terms in (2.34).

3. The stability analysis of the approximate problem

We now concentrate on the approximate problem:

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\triangle\psi + V(x,t)\psi, \quad x\in\Omega_R,\ 0<t\le T, \tag{3.1}$$

$$\psi\Big|_{t=0} = \psi^0(x), \quad x\in\Omega_R, \tag{3.2}$$

$$\frac{\partial\psi}{\partial r}\Big|_{|x|=R} = \Lambda_N\big(\psi|_{|x|=R}, \theta, t\big), \tag{3.3}$$

where

$$\begin{aligned}\Lambda_N\big(\psi|_{|x|=R},\theta,t\big) =& -\frac{1}{2\sqrt{\pi^3}}\int_0^t\int_0^{2\pi}\frac{\partial}{\partial\lambda}\Big(\psi(R,\xi,\lambda)e^{iV_\infty(\lambda-t)}\Big)\frac{S_0(t-\lambda)}{\sqrt{t-\lambda}}d\xi d\lambda \\ &-\sum_{n=1}^{N}\Big\{\frac{n}{R\pi}\int_0^{2\pi}\psi(R,\xi,t)\cos n(\xi-\theta)d\xi \\ &+\frac{1}{\sqrt{\pi^3}}\int_0^t\int_0^{2\pi}\frac{\partial}{\partial\lambda}\big(\psi(R,\xi,\lambda)\cos n(\xi-\theta)e^{iV_\infty(\lambda-t)}\big)\frac{S_n(t-\lambda)}{\sqrt{t-\lambda}}d\xi d\lambda\Big\}.\end{aligned} \tag{3.4}$$

Suppose that $\psi(r,\theta,t)$ is a solution of problem (3.1)–(3.3), then we have following lemma:

Lemma 3.1. *The following inequality holds:*

$$\mathrm{Im}\Big\{\int_0^t\int_0^{2\pi}\Lambda_N\big(\psi|_{|x|=R},\theta,\tau\big)\overline{\psi}(R,\theta,\tau)R\,d\theta\,d\tau\Big\}\ge 0, \qquad for \quad 0\le t\le T. \tag{3.5}$$

Proof: Let

$$\psi(R,\theta,t) = \frac{\alpha_{0,R}(t)}{2} + \sum_{n=1}^{\infty}\big(\alpha_{n,R}(t)\cos n\theta + \beta_{n,R}(t)\sin n\theta\big). \tag{3.6}$$

Substituting (3.6) into (3.4), we obtain

$$\begin{aligned}\Lambda_N\ \big(\psi|_{|x|=R},\theta,t\big) =& -\frac{1}{2\sqrt{\pi}}\int_0^t\frac{\partial}{\partial\lambda}\Big(\alpha_{0,R}(\lambda)e^{iV_\infty(\lambda-t)}\Big)\frac{S_0(t-\lambda)}{\sqrt{t-\lambda}}d\lambda \\ &-\sum_{n=1}^{N}\Big\{\Big[\frac{n}{R}\alpha_{n,R}(t)+\frac{1}{\sqrt{\pi}}\int_0^t\frac{\partial}{\partial\lambda}\big(\alpha_{n,R}(\lambda)e^{iV_\infty(\lambda-t)}\big)\frac{S_n(t-\lambda)}{\sqrt{t-\lambda}}d\lambda\Big]\cos n\theta \\ &+\Big[\frac{n}{R}\beta_{n,R}(t)+\frac{1}{\sqrt{\pi}}\int_0^t\frac{\partial}{\partial\lambda}\big(\beta_{n,R}(\lambda)e^{iV_\infty(\lambda-t)}\big)\frac{S_n(t-\lambda)}{\sqrt{t-\lambda}}d\lambda\Big]\sin n\theta\Big\}. \\ \equiv& \frac{W_0(\alpha_{0,R};t)}{2}+\sum_{n=1}^{N}\Big\{W_n(\alpha_{n,R};t)\cos n\theta+W_n(\beta_{n,R};t)\sin n\theta\Big\},\end{aligned} \tag{3.7}$$

with

$$W_n(f;t) = -\frac{n}{R}f(t) - \frac{1}{\sqrt{\pi}}\int_0^t \frac{\partial}{\partial\lambda}\big(f(\lambda)e^{iV_\infty(\lambda-t)}\big)\frac{S_n(t-\lambda)}{\sqrt{t-\lambda}}d\lambda, \quad \text{for } n=0,1,\cdots,N.$$

Then from (3.6) and (3.7), we have

$$\begin{aligned}
&\int_0^t\int_0^{2\pi}\Lambda_N\big(\psi|_{|x|=R},\theta,\tau\big)\overline{\psi}(R,\theta,\tau)Rd\theta d\tau \\
=&\pi R\int_0^t\left\{\frac{W_0(\alpha_{0,R};\tau)\overline{\alpha_{0,R}(\tau)}}{2}+\sum_{n=1}^N\Big[W_n(\alpha_{n,R};\tau)\overline{\alpha_{n,R}(\tau)}+W_n(\beta_{n,R};\tau)\overline{\beta_{n,R}(\tau)}\Big]\right\}d\tau.
\end{aligned} \tag{3.8}$$

On the other hand, we consider the following auxiliary problem on the domain $\{(r,t)|\, R\le r<+\infty,\ 0\le t\le T\}$ for $n=0,1,\cdots,N$:

$$\begin{aligned}
i\frac{\partial P_n}{\partial t} &= -\frac{1}{2}\Big(\frac{\partial^2 P_n}{\partial r^2}+\frac{1}{r}\frac{\partial P_n}{\partial r}-\frac{n^2}{r^2}P_n\Big)+V_\infty P_n, \quad R<r<+\infty,\ 0<t\le T, && (3.9)\\
P_n|_{r=R} &= \alpha_{n,R}, \quad 0<t\le T, && (3.10)\\
P_n|_{t=0} &= 0, \quad R\le r<+\infty, && (3.11)\\
P_n &\longrightarrow 0, \quad \text{when} \quad r\longrightarrow+\infty,\ 0<t\le T. && (3.12)
\end{aligned}$$

The problem (3.9)–(3.12) has been discussed in Section 2. From (2.32) we have

$$\frac{\partial P_n}{\partial r}\Big|_{r=R} = W_n(\alpha_{n,R};t). \tag{3.13}$$

Multiplying $r\overline{P_n(r,t)}$ on the equation (3.9) and taking the conjugation, we arrive at:

$$ir\overline{P}_n\frac{\partial P_n}{\partial t} = -\frac{1}{2}\left(\frac{\partial}{\partial r}\left(r\frac{\partial P_n}{\partial r}\right)\overline{P}_n-\frac{n^2}{r}P_n\overline{P}_n\right)+rV_\infty P_n\overline{P}_n, \tag{3.14}$$

$$-irP_n\frac{\partial\overline{P}_n}{\partial t} = -\frac{1}{2}\left(\frac{\partial}{\partial r}\left(r\frac{\partial\overline{P}_n}{\partial r}\right)P_n-\frac{n^2}{r}P_n\overline{P}_n\right)+rV_\infty P_n\overline{P}_n. \tag{3.15}$$

Combining (3.14) and (3.15), we get

$$ir\frac{\partial}{\partial t}|P_n(r,t)|^2 = -\frac{1}{2}\frac{\partial}{\partial r}\left(r\frac{\partial P_n}{\partial r}\right)\overline{P}_n+\frac{1}{2}\frac{\partial}{\partial r}\left(r\frac{\partial\overline{P}_n}{\partial r}\right)P_n. \tag{3.16}$$

Integrating (3.16) on $[R,+\infty)\times[0,t]$ and using (3.11), we have

$$i\int_R^{+\infty}|P_n(r,t)|^2rdr = i\ \mathrm{Im}\left\{R\int_0^t\frac{\partial P_n(R,\tau)}{\partial r}\overline{P}_n(R,\tau)d\tau\right\}.$$

Namely

$$0\le \mathrm{Im}\int_0^t\frac{\partial P_n(R,\tau)}{\partial r}\overline{P}_n(R,\tau)d\tau = \mathrm{Im}\int_0^t W_n(\alpha_{n,R};\tau)\overline{\alpha_{n,R}(\tau)}d\tau. \tag{3.17}$$

Similarly we can prove

$$0\le \mathrm{Im}\int_0^t W_n(\beta_{n,R};\tau)\overline{\beta_{n,R}(\tau)}d\tau. \tag{3.18}$$

Finally, the proof of Lemma 3.1 is completed in view of (3.8), (3.17) and (3.18). □

For the problem (3.1)–(3.3), we have the following stability estimate:

THEOREM 3.2. *Suppose that ψ is a solution of problem (3.1)–(3.3), the following stability estimate holds:*

$$\int_{\Omega_R} |\psi(x,t)|^2 dx \leq \int_{\Omega_R} |\psi^0(x)|^2 dx, \quad 0 \leq t \leq T. \tag{3.19}$$

Proof: Multiplying $\overline{\psi}$ on the equation (3.1) and taking the conjugation, we have

$$i\frac{\partial \psi}{\partial t}\overline{\psi} = -\frac{1}{2}\overline{\psi} \triangle \psi + V(x,t)\psi\overline{\psi}, \tag{3.20}$$

$$-i\frac{\partial \overline{\psi}}{\partial t}\psi = -\frac{1}{2}\psi \triangle \overline{\psi} + V(x,t)\overline{\psi}\psi. \tag{3.21}$$

In view of (3.20) and (3.21), we have

$$i\frac{\partial}{\partial t}|\psi|^2 = -\frac{1}{2}\overline{\psi} \triangle \psi + \frac{1}{2}\psi \triangle \overline{\psi}, \quad (x,t) \in \Omega_R \times [0,T]. \tag{3.22}$$

Integrating the equation (3.22) on the domain $\Omega_R \times [0,t]$ and integrating by parts, we obtain

$$\int_{\Omega_R} |\psi(x,t)|^2 dx = \int_{\Omega_R} |\psi^0(x)|^2 dx - \mathrm{Im}\left\{\int_0^t \int_0^{2\pi} \Lambda_N(\psi|_{|x|=R}, \theta, \tau)\overline{\psi(x,\tau)}|_{|x|=R} R d\theta d\tau\right\}.$$

Then the stability estimate (3.19) follows directly from Lemma 3.1. □

From the estimate (3.19), we obtain the uniqueness of the approximate problem (3.1)–(3.3) immediately.

COROLLARY 3.1. *The approximate problem (3.1)–(3.3) at most has one solution.*

4. The functions $\{S_n(t), n = 0, 1, \cdots\}$

The functions $\{S_n(t), n = 0, 1, \cdots\}$ are involved in the artificial boundary (2.34). Before we discuss the numerical solution of problem (1.1)–(1.3), we must calculate the functions $\{S_n(t), n = 0, 1, \cdots\}$ as a new class of special functions. By the definition of $S_n(t)$, we have:

$$S_n(t) = \frac{4\sqrt{t}}{\sqrt{\pi^3}} \int_0^{+\infty} \frac{e^{-\frac{i}{2}\mu^2 t}}{J_n^2(\mu R) + Y_n^2(\mu R)} \frac{d\mu}{\mu}.$$

From Fig. 4.1, 4.2 and 4.3, we can see that $S_n(t)$ are smooth. After discretizing the boundary condition (2.38), we need to calculate the summation

$$\sum_{k=1}^{m} \psi(R, \cdot, t_{m-k}) H_n(k),$$

where

$$t_k = k \triangle t, \text{ for } k = 1, \cdots, m,$$

and

$$H_n(k) = e^{-iV_\infty t_k} \int_{t_{k-1}}^{t_k} \frac{S_n(\lambda)}{\sqrt{\lambda}} d\lambda - e^{-iV_\infty t_{k+1}} \int_{t_k}^{t_{k+1}} \frac{S_n(\lambda)}{\sqrt{\lambda}} d\lambda. \tag{4.1}$$

As $k \to \infty$, $|H_n(k)|$ goes like $O((\frac{1}{k} + \triangle t)\sqrt{\frac{\triangle t}{k}})$ (see Fig. 4.4).

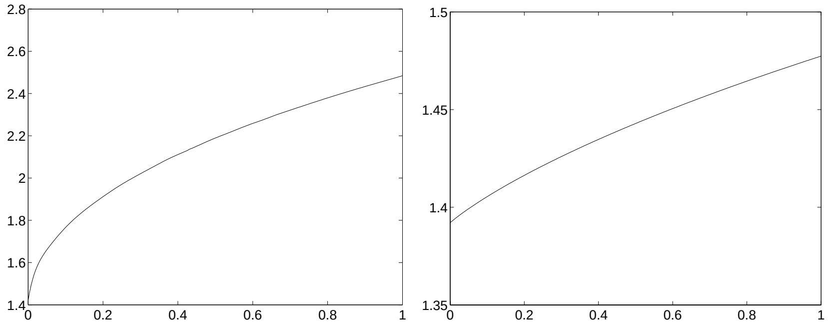

Fig. 4.1. *Re* $S_0(t)$ *and Im* $S_0(t)$

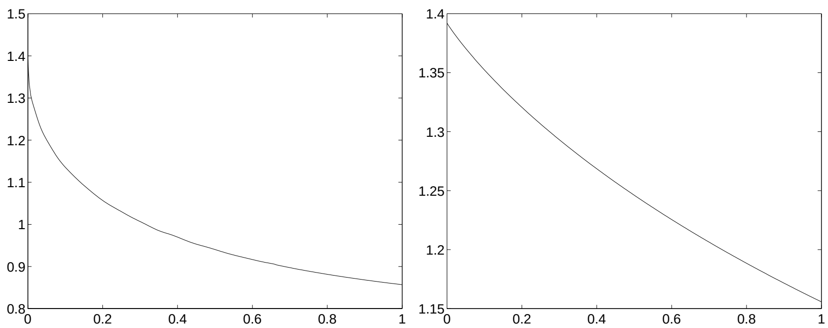

Fig. 4.2. *Re* $S_1(t)$ *and Im* $S_1(t)$

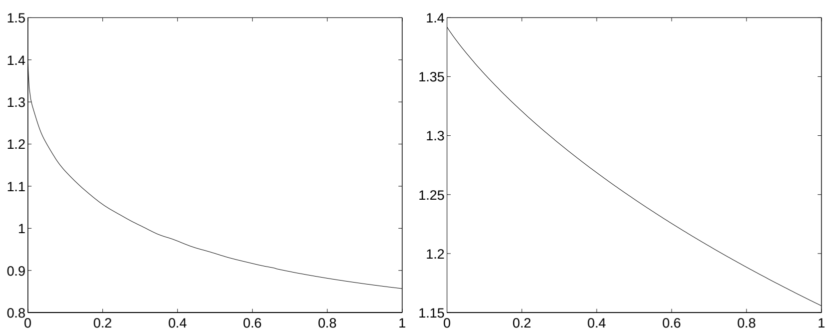

Fig. 4.3. *Re* $S_2(t)$ *and Im* $S_2(t)$

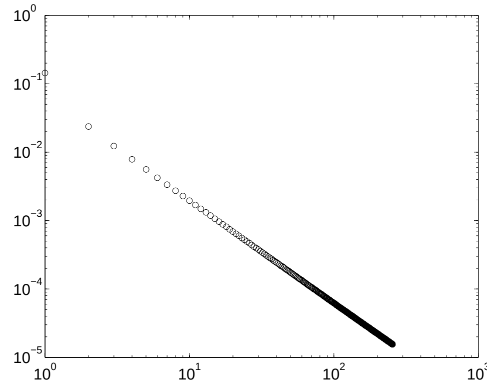

FIG. 4.4. *The graph of* $|H_0(k)|$ *in logarithmic scales. Here* $\triangle t = \frac{1}{256}$, $V_\infty = 0$.

5. A special case

Many popular potentials are independent on the radiation angle θ, such as Lennard-Jones potential and Coulomb potential. Therefore, in this section we consider this special case of problem (1.1)–(1.3). Suppose that the given potential $V(x,t)$ is symmetric, namely

$$V = V(r,t). \tag{5.1}$$

Let

$$\psi(r,\theta,t) = \frac{\psi_0(r,t)}{2} + \sum_{n=1}^{\infty}(\psi_n(r,t)\cos n\theta + \phi_n(r,t)\sin n\theta), \tag{5.2}$$

be the Fourier expansion of $\psi(r,\theta,t)$, the solution of problem (1.1)–(1.3), where $\psi_n(r,t)$ and $\phi_n(r,t)$ are defined in (2.3) and (2.4). From the above definitions, we can get directly

$$\lim_{r\to 0}\psi_n(r,t) = 0, \quad \text{for } n = 1,2,\cdots$$
$$\lim_{r\to 0}\phi_n(r,t) = 0, \quad \text{for } n = 1,2,\cdots$$

On the other hand, $\psi_0(r,t)$ can be considered as a function in Cartesian coordinates:

$$\psi_0(r,t) = \psi_0(\sqrt{x_1^2+x_2^2},t) \equiv \psi_0(x,t).$$

Then it is easy to get

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi_0}{\partial r}\right) = \triangle_x\psi_0, \qquad \text{for } \ r>0,$$

and

$$\lim_{r\to 0}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi_0}{\partial r}\right) = \triangle_x\psi_0(x,t)\big|_{|x|=0}.$$

It is reasonable that we can discretize the operator "$\triangle$" in Cartesian coordinates without singularity at $r = 0$. Therefore, $\psi_0(r,t)$ satisfies

$$i\frac{\partial \psi_0}{\partial t} = -\frac{1}{2}\left(\frac{\partial^2 \psi_0}{\partial r^2} + \frac{1}{r}\frac{\partial \psi_0}{\partial r}\right) + V(r,t)\psi_0, \quad 0 < r < +\infty, 0 < t \le T, \tag{5.3}$$

$$\psi_0|_{t=0} = \psi_0^0(r), \quad 0 \le r < +\infty, \tag{5.4}$$

$$i\frac{\partial \psi_0}{\partial t}\Big|_{r=0} = \left(-\frac{1}{2}\triangle \psi_0 + V\psi_0\right)\Big|_{r=0}, \quad 0 < t \le T, \tag{5.5}$$

$$\psi_0 \longrightarrow 0, \quad \text{when} \quad r \longrightarrow +\infty,\ 0 < t \le T, \tag{5.6}$$

$\psi_n(r,t)(n = 1, 2, \cdots)$ satisfy

$$i\frac{\partial \psi_n}{\partial t} = -\frac{1}{2}\left(\frac{\partial^2 \psi_n}{\partial r^2} + \frac{1}{r}\frac{\partial \psi_n}{\partial r} - \frac{n^2}{r^2}\psi_n\right) + V(r,t)\psi_n, 0 < r < +\infty, 0 < t \le T, \tag{5.7}$$

$$\psi_n|_{t=0} = \psi_n^0(r), \quad 0 \le r < +\infty, \tag{5.8}$$

$$\psi_n|_{r=0} = 0, \quad 0 < t \le T, \tag{5.9}$$

$$\psi_n \longrightarrow 0, \quad \text{when} \quad r \longrightarrow +\infty,\ 0 < t \le T, \tag{5.10}$$

$\phi_n(r,t)(n = 1, 2, \cdots)$ satisfy

$$i\frac{\partial \phi_n}{\partial t} = -\frac{1}{2}\left(\frac{\partial^2 \phi_n}{\partial r^2} + \frac{1}{r}\frac{\partial \phi_n}{\partial r} - \frac{n^2}{r^2}\phi_n\right) + V(r,t)\phi_n, 0 < r < +\infty, 0 < t \le T, \tag{5.11}$$

$$\phi_n|_{t=0} = \phi_n^0(r), \quad 0 \le r < +\infty, \tag{5.12}$$

$$\phi_n|_{r=0} = 0, \quad 0 < t \le T, \tag{5.13}$$

$$\phi_n \longrightarrow 0, \quad \text{when} \quad r \longrightarrow +\infty,\ 0 < t \le T, \tag{5.14}$$

where

$$\psi_n^0(r) = \frac{1}{\pi}\int_0^{2\pi} \psi^0(r,\theta)\cos(n\theta)d\theta, \quad n = 0, 1, \cdots \tag{5.15}$$

$$\phi_n^0(r) = \frac{1}{\pi}\int_0^{2\pi} \phi^0(r,\theta)\sin(n\theta)d\theta, \quad n = 1, 2, \cdots \tag{5.16}$$

Now the two dimensional problem (1.1)–(1.3) is reduced to a series of one dimensional problems (5.3)–(5.6), (5.7)–(5.10) and (5.11)–(5.14). By the condition (1.2), we know that

$$\psi_n^0(r) = 0, \quad \text{and} \quad \phi_n^0(r) = 0, \quad \text{when} \quad r \ge R, \tag{5.17}$$

Using (2.32) and (2.33), the problems (5.3)–(5.6), (5.7)–(5.10) and (5.11)–(5.14) are equivalent to the following problems on a bounded domain:

$$i\frac{\partial \psi_0}{\partial t} = -\frac{1}{2}\left(\frac{\partial^2 \psi_0}{\partial r^2} + \frac{1}{r}\frac{\partial \psi_0}{\partial r}\right) + V(r,t)\psi_0,\ r \in (0,R), \quad t > 0, \tag{5.18}$$

$$\frac{\partial \psi_0}{\partial r}\Big|_{r=R} = -\frac{1}{\sqrt{\pi}}\int_0^t \frac{\partial}{\partial \lambda}\left(\psi_0(R,\lambda)e^{iV_\infty(\lambda - t)}\frac{S_0(t-\lambda)}{\sqrt{t-\lambda}}\right)d\lambda,\ t > 0, \tag{5.19}$$

$$i\frac{\partial \psi_0}{\partial t}\Big|_{r=0} = \Big(-\frac{1}{2}\triangle \psi_0 + V\psi_0\Big)\Big|_{r=0}, \quad 0 < t \le T, \tag{5.20}$$

$$\psi_0\big|_{t=0} = \psi_0^0(r), \quad r \in [0,R], \tag{5.21}$$

$$i\frac{\partial\psi_n}{\partial t} = -\frac{1}{2}\left(\frac{\partial^2\psi_n}{\partial r^2} + \frac{1}{r}\frac{\partial\psi_n}{\partial r} - \frac{n^2}{r^2}\psi_n\right) + V(r,t)\psi_n,\ r\in(0,R),\quad t>0, \tag{5.22}$$

$$\frac{\partial\psi_n}{\partial r}\Big|_{r=R} = -\frac{n}{R}\psi_n(R,t) - \frac{1}{\sqrt{\pi}}\int_0^t \frac{\partial}{\partial\lambda}\left(\psi_n(R,\lambda)e^{iV_\infty(\lambda-t)}\frac{S_n(t-\lambda)}{\sqrt{t-\lambda}}\right)d\lambda,\ t>0, \tag{5.23}$$

$$\psi_n\big|_{r=0} = 0,\quad 0<t\le T, \tag{5.24}$$

$$\psi_n\big|_{t=0} = \psi_n^0(r),\quad r\in[0,R], \tag{5.25}$$

$$i\frac{\partial\phi_n}{\partial t} = -\frac{1}{2}\left(\frac{\partial^2\phi_n}{\partial r^2} + \frac{1}{r}\frac{\partial\phi_n}{\partial r} - \frac{n^2}{r^2}\phi_n\right) + V(r,t)\phi_n,\ r\in(0,R),\quad t>0, \tag{5.26}$$

$$\frac{\partial\phi_n}{\partial r}\Big|_{r=R} = -\frac{n}{R}\phi_n(R,t) - \frac{1}{\sqrt{\pi}}\int_0^t \frac{\partial}{\partial\lambda}\left(\phi_n(R,\lambda)e^{iV_\infty(\lambda-t)}\frac{S_n(t-\lambda)}{\sqrt{t-\lambda}}\right)d\lambda,\ t>0, \tag{5.27}$$

$$\phi_n\big|_{r=0} = 0,\quad 0<t\le T, \tag{5.28}$$

$$\phi_n\big|_{t=0} = \phi_n^0(r),\quad r\in[0,R]. \tag{5.29}$$

6. Numerical examples

In this section, we give two numerical examples.

Example 1. First, we consider a simple one:

$$\begin{aligned} i\frac{\partial\psi}{\partial t} &= -\frac{1}{2}\Big(\frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2}\Big) + V(r,t)\psi,\quad r>0,\ t>0 && (6.1)\\ \psi\big|_{t=0} &= \psi^0(r),\quad r\ge 0, && (6.2)\\ \lim_{r\to 0} r\frac{\partial\psi}{\partial r} &= 0,\quad t>0, && (6.3)\\ \psi &\longrightarrow 0,\quad \text{when}\quad r\longrightarrow +\infty,\ t\ge 0, && (6.4)\end{aligned}$$

where

$$V(r,t) = \begin{cases} \sin(2\pi r), & r\in[0,1],\\ 0, & \text{otherwise,}\end{cases}$$

$$\psi^0(r) = \begin{cases} 1+\cos(\pi r) + i(\cos(2\pi r)-1), & r\in[0,1],\\ 0, & \text{otherwise,}\end{cases}$$

(see Fig. 6.1-6.2). That means the initial condition and the potential are independent of θ, so is the solution of this problem. Therefore, we can only use one component in our numerical solution, namely we need only solve (5.18)–(5.21). The results are given in Fig. 6.3. The numerical solution mimics the exact solution very well.

Example 2. Then we consider a Cauchy problem for the Schrödinger equation in the absence of a potential (i.e. $V(x)=0$):

$$\begin{aligned} i\frac{\partial\psi}{\partial t} &= -\frac{1}{2}\Big(\frac{\partial^2\psi}{\partial r^2} + \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2}\Big),\ r>0,\ \theta\in[0,2\pi],\ t>0, && (6.5)\\ \psi\big|_{t=0} &= \psi^0(r,\theta),\quad r\ge 0,\ \theta\in[0,2\pi], && (6.6)\\ \lim_{r\to 0} r\frac{\partial\psi}{\partial r} &= 0,\quad \theta\in[0,2\pi],\ t>0, && (6.7)\\ \psi &\longrightarrow 0,\quad \text{when}\quad r\longrightarrow +\infty,\ \theta\in[0,2\pi],\ t\ge 0, && (6.8)\end{aligned}$$

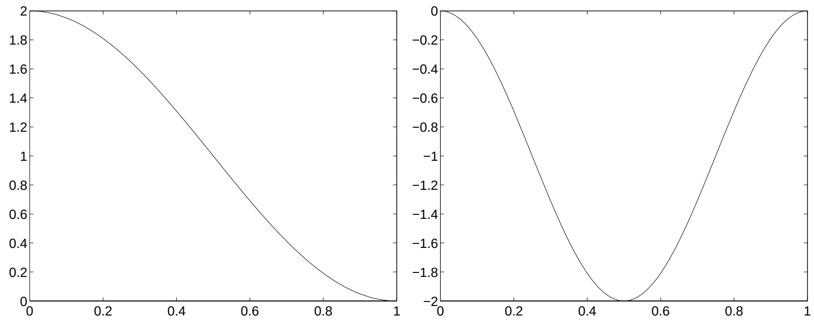

FIG. 6.1. *Re* $\psi^0(r)$ *and Im* $\psi^0(r)$

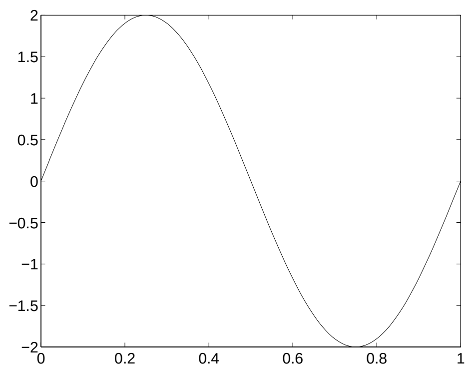

FIG. 6.2. *Potential function* $V(r)$

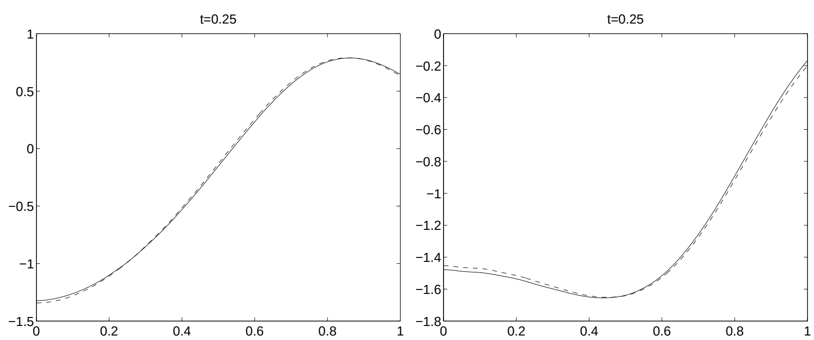

FIG. 6.3. *Comparison of the exact solution and our numerical solution at time* $t = 0.25$. *The solid line is the exact solution, the dash line is our numerical solution. We use the Crank-Nicolson method in our simulation. The left one is the real part, the right one is the imaginary part. Here* $R = 1$, $\triangle t = \triangle r = \frac{1}{256}$. *We let* $N = 0$ *(refer to (2.38)), that means we only use the first item in (2.34).*

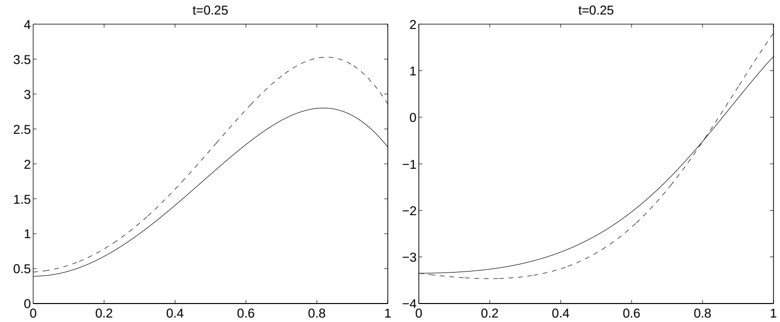

FIG. 6.4. *Comparison of the exact solution and our numerical solution at time $t = 0.25$. The dash line is the exact solution, the solid one is our numerical solution. We use the Crank-Nicolson method in our simulation. The left one is the real part, the right one is the imaginary part. Here we let $R = 1$, $\triangle t = \triangle r = \frac{1}{256}$, $N = 0$ (refer to (2.38)).*

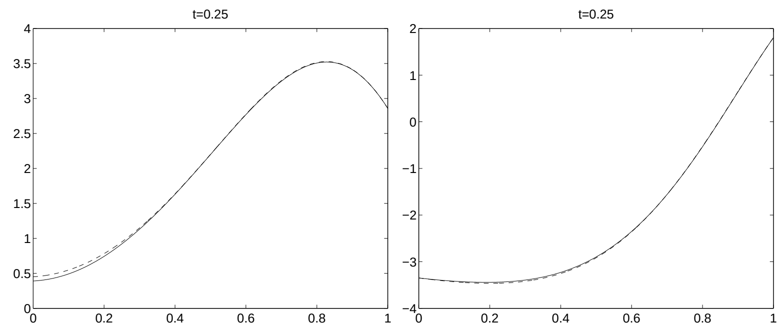

FIG. 6.5. *Comparison of the exact solution and our numerical solution at time $t = 0.25$. The dash line is the exact solution, the solid one is our numerical solution. We use the Crank-Nicolson method in our simulation. The left one is the real part, the right one is the imaginary part. Here we let $R = 1$, $\triangle t = \triangle r = \frac{1}{256}$, $N = 1$ (refer to (2.38)).*

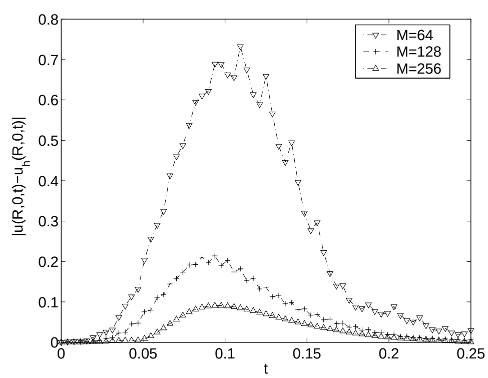

FIG. 6.6. *The difference between the exact solution and our numerical solution at artificial boundary Γ_R for different meshes. Here we let $R = 1$, $\triangle r = \triangle t = \frac{1}{M}$, $N = 1$ (refer to (2.38)).*

where

$$\psi^0(r,\theta) = \frac{e^{2ik_x r\cos\theta + 2ik_y r\sin\theta - \frac{(r\cos\theta)^2}{2\alpha_x} - \frac{(r\sin\theta)^2}{2\alpha_y}}}{\sqrt{\alpha_x\alpha_y}}.$$

The exact solution is

$$\psi(r,\theta,t) = \frac{e^{2ik_x(r\cos\theta - k_x t) + 2ik_y(r\sin\theta - k_y t) - \frac{(r\cos\theta - 2k_x t)^2}{2(\alpha_x + it)} - \frac{(r\sin\theta - 2k_y t)^2}{2(\alpha_y + it)}}}{\sqrt{\alpha_x + it}\sqrt{\alpha_y + it}}.$$

We let $\alpha_x = \alpha_y = 0.04$, $k_x = -k_y = 1$. Here the initial condition depends on θ. If we only use one component, i.e. $N = 0$ for (5.22)–(5.25), we can not get a satisfied solution (see Fig. 6.4). But if we use three components, i.e. $N = 0$ and 1 for (5.22)–(5.25) and $N = 1$ for (5.26)–(5.29), we can get a very good approximation (see Fig. 6.5). The comparison of the exact solution and our numerical solution at time $t = 0.25$ is give in Fig. 6.6.

7. Conclusion

In this paper, we provide a kind of exact artificial boundary condition for the numerical solution of Schrödinger equation on unbounded domains in two-dimensional cases. First, we introduce an artificial boundary, then we get a initial-boundary problem on a finite domain enclosed by the artificial boundary which is equivalent to the original problem. In addition, after we use the variables separation technique and some properties of Bessel functions, we can obtain the exact artificial boundary condition in a very simple formula. Then we can get a series of approximate artificial boundary conditions. Furthermore, we proved the well-posedness of the approximate problem (3.1)–(3.3). As the kernels of our ABCs have only weak singularities, it is easy to integrate them. In our numerical simulation, from the Fig. 4.4, we can see that the kernel in this convolution decays very fast. By this property, we can truncate the convolution to save the calculation in long time evolution problems. When the potential function is independent of the radiant angle θ, the problem can be reduced to a series of one-dimensional problems. That can reduce the computation complexity greatly. Our numerical examples show that we can get good numerical solutions with no numerical reflections using our artificial boundary conditions.

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