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ABSTRACT

The photon diffusion equation is solved making use of the Born series for the Robin boundary condition. We develop a general theory for arbitrary domains with smooth enough boundaries and explore the convergence. The proposed Born series is validated by numerical calculation in the three-dimensional half space. It is shown that in this case, the Born series converges regardless the value of the impedance term in the Robin boundary condition.

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I. INTRODUCTION

Diffusion is often seen in different subfields of science and engineering. In particular, light propagation in turbid media such as biological tissue is governed by the diffusion equation except near sources and boundaries.¹¹ There are scattering and absorption in the medium, and they are characterized by the diffusion and absorption coefficients in the diffusion equation or the photon diffusion equation emphasizing the existence of the absorption term. In addition to its importance in natural science, diffusion in random media has been utilized in medicine.²¹ Diffuse optical tomography (DOT) is a near-infrared version of X-ray computed tomography,⁵ for which inverse problems are to determine, from boundary measurements, the diffusion coefficient and the absorption coefficient.^{1,3} Brain activity has been investigated by near-infrared spectroscopy from boundary measurements of diffuse light.¹⁰

At the depth of about ten times the transport mean free path, the energy density of light, which is governed by the Maxwell equations, starts to obey the diffusion equation via the mesoscopic regime of the radiative transport equation.^{19,22} Therefore, for highly scattering media such as biological tissue, the diffusion regime becomes dominant. Hence, it is common to assume that the diffusion regime spans the whole domain including the boundary. Then, the energy density of light in the medium is obtained as the solution to the photon diffusion equation with the Robin boundary condition.

In this paper, we consider the Born sequence for the Robin boundary condition and derive the solution to the diffusion equation as a series. The convergence of the Born series is tested when the spatial domain is a three dimensional half space. More precisely, for a diffusion equation with a homogeneous diffusion coefficient and an absorption coefficient given in the half space over some finite time interval with the Robin boundary condition, we tested the convergence of the Born series for the Poisson kernel when we treat the Robin boundary condition as a perturbation of the Neumann boundary condition. A striking result given later in Sec. V (see Remark V.2) is that this Born series converges even when the homogeneous impedance term of the Robin boundary condition is not small.

The rest of this paper is organized as follows. In Sec. II, we will discuss the efficiency of the so-called extrapolated boundary condition, which has been used in the study of optical tomography. This boundary condition was introduced to give an approximate solution in a concise way for the initial boundary value problem for the aforementioned diffusion equation with the Robin boundary condition. We show that the efficiency of this boundary condition is limited, which led us to our study given in this paper. Section III is devoted to a general study of the Born approximation. Then, based on this general study, we define in Sec. IV the Born approximation for the Poisson kernel in the half

space and a slab domain over some finite time interval. Furthermore, we discuss its convergence of the Born approximation for the Poisson kernel in the half space over some finite time interval in Sec. V. In Sec. VI, we tested the numerical performance of the Born approximation for the Poisson kernel in the half space over some finite time interval. The last section is for concluding remarks. Appendixes A–C give some supplementary arguments and facts that are better to be separated from the main part of this paper to clarify the points of arguments.

II. ANALYTICAL SOLUTION AND EXTRAPOLATED BOUNDARY

Let us consider the domain $\Omega = \mathbb{R}_+^3$, where $\mathbb{R}_+^3 = \{x \in \mathbb{R}^3; x_3 > 0\}$. The boundary, i.e., the x_1 - x_2 plane, is denoted by $\partial\Omega$. We will find an expression for u that satisfies

$$\begin{cases} (\partial_t - \gamma\Delta + b)u = 0, & (x, t) \in \Omega_T, \\ \gamma\partial_\nu u + \beta u = \delta(x_1 - y_1)\delta(x_2 - y_2)\delta(t - s), & (x, t) \in \partial\Omega_T, \\ u = 0, & x \in \Omega, \quad t = 0, \end{cases} \quad (1)$$

where in the Robin boundary condition, $\partial_\nu = \nu \cdot \nabla$ with ν as the unit normal of $\partial\Omega$ directed into the exterior of Ω .

Considerable efforts have been paid to derive concise solution formulae for the diffusion equation.^{2,8,14} Among such efforts, the extrapolated boundary is a *fudged-up* boundary (Chap. 5 in the book by Duderstadt and Hamilton⁶) placed in an infinite medium obtained by removing the true boundary. Although it is not easy to mathematically justify the validity of the extrapolated boundary condition, this boundary condition has been successfully used for light propagation in biological tissue.^{4,12,17,19}

The diffusion equation with the extrapolated boundary condition is described as the following initial value problem for $u_{\text{EBC}}(x, t)$:

$$\begin{cases} (\partial_t - \gamma\Delta + b)u_{\text{EBC}} = \delta(x_1 - y_1)\delta(x_2 - y_2)[\delta(x_3) - \delta(x_3 + 2\ell)]\delta(t - s), \\ u_{\text{EBC}} = 0, \quad x \in \mathbb{R}^3, \quad t = 0. \end{cases} \quad (x, t) \in \mathbb{R}^3 \times (0, T), \quad (2)$$

Here, the ratio $\ell = \gamma/\beta$ is called the extrapolation distance. u_{EBC} restricted to Ω will be considered to approximate the solution u of (1). When ℓ is close to 0, the boundary $\partial\Omega$ is almost purely absorbing, and the purely reflecting boundary is achieved in the limit $\ell \rightarrow \infty$. We remark that sometimes the source is placed inside the medium with the source term given by $\delta(x_1 - y_1)\delta(x_2 - y_2)[\delta(x_3 - d) - \delta(x_3 + 2\ell - d)]\delta(t - s)$, where d is about the transport mean free path.¹⁷

We briefly examine the performance of approximating u by $u_{\text{EBC}}(x, t)$ restricting to Ω . In Appendix A, we explicitly calculate the solution to (1) in the half space. We put

$$y_1 = y_2 = s = 0. \quad (3)$$

Then, the exact solution to (1) at $x_1 = x_2 = 0$ for $x_3 > 0, t \geq 0$ is given by

$$u(x, t) = u(x_3, t) = \frac{2e^{-bt}}{4\pi\gamma t} \left[\frac{e^{-\frac{x_3^2}{4\gamma t}}}{\sqrt{4\pi\gamma t}} - \frac{\beta}{2\gamma} e^{\frac{\ell}{\gamma}(x_3 + \beta t)} \operatorname{erfc}\left(\frac{x_3 + 2\beta t}{\sqrt{4\gamma t}}\right) \right], \quad (4)$$

where the complementary error function $\operatorname{erfc}(\xi)$, $\xi \in \mathbb{R}$, is defined as

$$\operatorname{erfc}(\xi) = \frac{2}{\sqrt{\pi}} \int_{\xi}^{\infty} e^{-s^2} ds.$$

Furthermore, we obtain

$$u_{\text{EBC}}(x_3, t) = \frac{e^{-bt}}{(4\pi\gamma t)^{3/2}} \left(e^{-\frac{x_3^2}{4\gamma t}} - e^{-\frac{(x_3 + 2\gamma/\beta)^2}{4\gamma t}} \right). \quad (5)$$

Let us numerically compare u and the restriction of u_{EBC} to Ω . First of all noticing $\operatorname{erfc}(\xi) = \frac{1}{\sqrt{\pi}} e^{-\xi^2} (\xi^{-1} + O(\xi^{-3}))$ for large ξ , we have

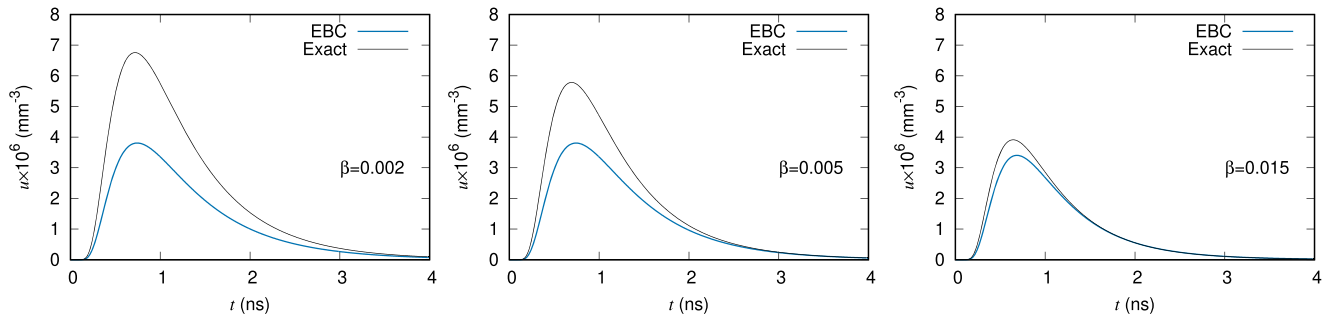


FIG. 1. The energy density u is plotted at $x_3 = 20$ mm as a function of t for, from the left to right, $\beta = 0.002$ mm/ps, $\beta = 0.005$ mm/ps, and $\beta = 0.015$ mm/ps, respectively. In each panel, $u(x_3, t)$ and $u_{\text{EBC}}(x_3, t)$ are compared.

$$\left| \frac{u_{\text{EBC}}(x_3, t) - u(x_3, t)}{u(x_3, t)} \right| = \frac{1 + e^{-\frac{x_3 + \gamma t}{\beta t}} - \frac{\beta}{\gamma} \sqrt{4\gamma t} (\xi^{-1} + O(\xi^{-3}))}{2 - \frac{\beta}{\gamma} \sqrt{\frac{\gamma t}{\pi}} (\xi^{-1} + O(\xi^{-3}))},$$

where $\xi = (x_3 + 2\beta t)/\sqrt{4\gamma t}$. Therefore, we obtain $\lim_{x_3 \rightarrow \infty} |(u_{\text{EBC}} - u)/u| = 1/2 \neq 0$ although $\lim_{t \rightarrow \infty} |(u_{\text{EBC}} - u)/u| = \lim_{\beta \rightarrow \infty} |(u_{\text{EBC}} - u)/u| = 0$.

Next, we set

$$\gamma = 0.06 \text{ mm}^2/\text{ps}, \quad b = 0.001 \text{ ps}^{-1}, \quad T = 4 \text{ ns}, \quad x_3 = 20 \text{ mm}. \quad (6)$$

In Fig. 1, we compare $u(x_3, t)$ in (4) and $u_{\text{EBC}}(x_3, t)$ in (5). When β is small, the agreement is not good. As β becomes larger, u_{EBC} approaches the exact solution $u(x_3, t)$.

III. GENERAL THEORY FOR BORN SERIES

In this section, a general scheme is given to define the Born series for the initial boundary value problem for the diffusion equation with the Robin boundary condition. The impedance term [i.e., βu in (1)] in the Robin boundary condition is considered as a perturbation for the Born series.

Throughout this section, let Ω be a domain in $\mathbb{R}^n$ ($n = 2, 3$) and $\partial\Omega$ be the boundary of Ω which is of C^2 class. For simplicity of description, we only describe our scheme for $n = 3$. We define

$$\Omega_T = \Omega \times (0, T), \quad \partial\Omega_T = \partial\Omega \times (0, T), \quad T > 0.$$

Let $\gamma = (\gamma_{ij})$ and b be the diffusion coefficient and the absorption coefficient that are bounded measurable in Ω , i.e., $\gamma, b \in L^\infty(\Omega)$. We assume that there exists a positive constant δ such that

$$\begin{cases} b \geq \delta, \\ \sum_{i,j=1}^3 \gamma_{ij}(x) \xi_i \xi_j \geq \delta \sum_{i=1}^3 \xi_i^2 \text{ for any } \xi = (\xi_1, \xi_2, \xi_3) \in \mathbb{R}^3 \end{cases} \quad (7)$$

almost everywhere in Ω . Now, we consider the following initial boundary value problem for the diffusion equation for the energy density $u(x, t)$:

$$\begin{cases} (\partial_t - \nabla \cdot \gamma \nabla + b)u = f, & (x, t) \in \Omega_T, \\ \gamma \partial_\nu u + \beta u = g, & (x, t) \in \partial\Omega_T, \\ u = 0, & x \in \Omega, \quad t = 0, \end{cases} \quad (8)$$

where $f = f(x, t)$ is the internal source, $g = g(x, t)$ is the boundary source, and β is a positive bounded measurable function on $\partial\Omega$, i.e., $\beta \in L^\infty(\partial\Omega)$. For the simplicity of description, we assume $\gamma = \gamma(x)I$ with scalar function $\gamma(x) \in L^\infty(\Omega)$ abusing the notation γ and the 3×3 identity matrix I .

Remark III.1. We can include the incident beam $h(x)$ in the initial condition of (8). By Duhamel's principle, however, it can reduce to the case $h = 0$.

In order to give the definition of the weak solution to (8), we first introduce L^2 -Sobolev spaces and related function spaces. Let $H^1(\Omega)$ be the real L^2 Sobolev space of order 1 in Ω , and we denote its dual space by $H^1(\Omega)^*$. Similarly, we let $H^{1/2}(\partial\Omega)$ be the real L^2 Sobolev space of order 1/2 on $\partial\Omega$ and denote its dual space by $H^{-1/2}(\partial\Omega)$. Define the trace operator $\Lambda : H^1(\Omega) \ni \psi \mapsto \psi|_{\partial\Omega} \in H^{1/2}(\partial\Omega)$. Here, we can consider $\Lambda\psi \in H^{-1/2}(\partial\Omega)$ because $H^{1/2}(\partial\Omega) \subset H^{-1/2}(\partial\Omega)$. We will use the pairings $\langle \cdot, \cdot \rangle_\Omega$ and $\langle \cdot, \cdot \rangle_{\partial\Omega}$ for the pairs $(H^1(\Omega), H^1(\Omega)^*)$ and $(H^{1/2}(\partial\Omega), H^{-1/2}(\partial\Omega))$, respectively. Furthermore, for any real Hilbert space E , $L^2((0, T); E)$ denotes the set of all E valued L^2 functions over the time interval $(0, T)$. We will denote its norm by $\|\cdot\|_{L^2((0, T); E)}$. Throughout the paper, $W((0, T))$ denotes the space defined as

$$W((0, T)) := \{u = u(t) := u(\cdot, t) \in L^2((0, T); H^1(\Omega)); \partial_t u \in L^2((0, T); H^1(\Omega)^*)\},$$

equipped with the norm

$$\|u\|_{W((0, T))}^2 := \int_0^T (\|u(t)\|_{H^1(\Omega)}^2 + \|\partial_t u(t)\|_{H^1(\Omega)^*}^2) dt.$$

We define the weak solution u to (8) as follows.

Definition III.2. Let $f = f(t) := f(\cdot, t) \in L^2((0, T); H^1(\Omega))$ and $g = g(t) := g(\cdot, t) \in L^2((0, T); H^{-1/2}(\partial\Omega))$. Then, $u \in W((0, T))$ is called the weak solution to (8) if it satisfies $u(0) = 0$ and

$$\begin{aligned} \int_0^T \{ \langle \partial_t u, \varphi(t) \rangle_\Omega + \langle \gamma \nabla u(t), \nabla \varphi(t) \rangle_\Omega + \langle bu(t), \varphi(t) \rangle_\Omega + \langle \beta \Lambda u(t), \Lambda \varphi(t) \rangle_{\partial\Omega} \} dt \\ = \int_0^T \langle f(t), \varphi(t) \rangle_\Omega dt + \int_0^T \langle g(t), \Lambda \varphi(t) \rangle_{\partial\Omega} dt \end{aligned} \quad (9)$$

for any $\varphi = \varphi(t) := \varphi(\cdot, t) \in Z((0, T)) := \{\varphi, \partial_t \varphi \in L^2((0, T); H^1(\Omega)), \varphi(T) = 0\}$.

A. Operators A, A_0

Let us consider the following sesquilinear forms:

$$\begin{cases} a(v, w) := \int_\Omega (\gamma \nabla v \cdot \nabla w + bvw) + \int_{\partial\Omega} \beta vw, \\ a_0(v, w) := \int_\Omega (\gamma \nabla v \cdot \nabla w + bvw), \end{cases} \quad (10)$$

where $v, w \in H^1(\Omega)$. By using $\gamma, b \in L^\infty(\Omega)$, (7), and the positivity of $\beta \in L^\infty(\partial\Omega)$, we can show that $a(v, w), a_0(v, w)$ are bounded, symmetric, and positive bilinear forms.²⁰ That is,

$$\begin{cases} |a(v, w)|, |a_0(v, w)| \leq C_1 \|v\|_{H^1(\Omega)} \|w\|_{H^1(\Omega)} \text{ (bounded)}, \\ a(v, w) = a(w, v), a_0(v, w) = a_0(w, v) \text{ (symmetric)}, \\ a(v, v), a_0(v, v) \geq C_2 \|v\|_{H^1(\Omega)}^2 \text{ (positive)} \end{cases} \quad (11)$$

for any $v, w \in H^1(\Omega)$ with some positive constants C_1, C_2 independent of v, w . Here, we denoted the $H^1(\Omega)$ norm of $v \in H^1(\Omega)$ by $\|v\|_{H^1(\Omega)}$. For $v \in H^1(\Omega)$ and $v_0 \in H^1(\Omega)$, let $\Psi \in H^1(\Omega)^*$ and $\Psi_0 \in H^1(\Omega)^*$ be such that for any $\phi \in H^1(\Omega)$, $\Psi(\phi) = a(v, \phi)$ and $\Psi_0(\phi) = a_0(v_0, \phi)$, respectively. Then, define A and A_0 by $Av = \Psi$ and $A_0 v_0 = \Psi_0$, respectively. From the properties (11), we see that A and A_0 are isomorphisms from $H^1(\Omega)$ to $H^1(\Omega)^*$.²⁰

Now, we define $F = F(t) \in L^2((0, T); H^1(\Omega)^*)$ by

$$\langle F(t), w \rangle_\Omega = \langle f(t), w \rangle_\Omega + \langle g(t), \Lambda w \rangle_{\partial\Omega}, \text{ a.e. } t \in (0, T) \quad (12)$$

for any $w \in H^1(\Omega)$. It is easy to show that the norm $\|F\|_{L^2((0, T); H^1(\Omega)^*)}$ of F has the estimate

$$\|F\|_{L^2((0, T); H^1(\Omega)^*)} \leq C(\|f\|_{L^2((0, T); H^1(\Omega)^*)} + \|g\|_{L^2((0, T); H^{-1/2}(\partial\Omega))}) \quad (13)$$

with some general constant $C > 0$.

Since

$$\int_0^T \langle \partial_t u(t), \varphi(t) \rangle_\Omega dt + \int_0^T \langle u(t), \partial_t \varphi(t) \rangle_\Omega dt = \langle u(T), \varphi(T) \rangle_\Omega - \langle u(0), \varphi(0) \rangle_\Omega$$

for any $u = u(t) := u(\cdot, t) \in W((0, T))$ and $\varphi = \varphi(t) := \varphi(\cdot, t) \in L^2((0, T); H^1(\Omega))$ such that $\partial_t \varphi \in L^2((0, T); H^1(\Omega))$, the weak solution $u = u(t) := u(\cdot, t)$ to (8) in Definition III.2 is equivalent to $u \in W((0, T))$ that satisfies

$$\partial_t u + Au = F \text{ in } L^2((0, T); H^1(\Omega)^*), \quad u(0) = 0 \text{ in } H^1(\Omega)^*. \quad (14)$$

Similarly, the definition of the weak solution $u = u(t) := u(\cdot, t)$ to (8) with $\beta = 0$ is equivalent to the definition given by

$$\partial_t u + A_0 u = F \text{ in } L^2((0, T); H^1(\Omega)^*), \quad u(0) = 0 \text{ in } H^1(\Omega)^*. \quad (15)$$

The fundamental theorem for the well-posedness of the weak solution to either (8) or (8) with $\beta = 0$ is as follows.

Theorem III.3 (Theorem 26.1 of Ref. 20). *Let $f \in L^2((0, T); H^1(\Omega)^*)$ and $g \in L^2((0, T); H^{-1/2}(\partial\Omega))$. Then, there exists a unique solution $u = u(t) := u(\cdot, t) \in W((0, T))$ to either (8) or (8) with $\beta = 0$. Furthermore, it satisfies $u \in C^0([0, T]; L^2(\Omega))$ and the estimate*

$$\|u\|_{W((0, T))} \leq C(\|f\|_{L^2((0, T); H^1(\Omega)^*)} + \|g\|_{L^2((0, T); H^{-1/2}(\partial\Omega))}) \quad (16)$$

with some general constant $C > 0$.

Based on this theorem, we will define the solution operator S_0 as follows.

Definition III.4. Define the Green operator S_0 and Poisson operator P_0 of (15) by $S_0 f = u$ and $P_0 g = u$, where $u \in W((0, T))$ is the solution to (15) with $g = 0$ and $f = 0$, respectively.

We note by (16) that

$$\|S_0 f\|_{W((0, T))} \leq C\|f\|_{L^2((0, T); H^1(\Omega)^*)}$$

holds for a general constant $C > 0$.

B. Born sequence

Let B be an operator $B : L^2((0, T); H^1(\Omega)) \rightarrow L^2((0, T); H^1(\Omega)^*)$ defined by

$$\int_0^T \langle Bv(t), w(t) \rangle_\Omega dt = \int_0^T \langle \beta \Lambda v(t), \Lambda w(t) \rangle_{\partial\Omega} dt \quad (17)$$

for $v = v(t) := v(\cdot, t)$, $w = w(t) := w(\cdot, t) \in L^2((0, T); H^1(\Omega))$.

Observe that by using the boundedness of the trace operator $\Lambda : H^1(\Omega) \rightarrow H^{1/2}(\partial\Omega)$, we have for any $v, w \in H^1(\Omega)$,

$$|\langle \beta \Lambda v, \Lambda w \rangle_{\partial\Omega}| \leq C\|\beta\|_{L^\infty(\partial\Omega)}\|v\|_{H^1(\Omega)}\|w\|_{H^1(\Omega)} \quad (18)$$

with some general constant $C > 0$. This immediately implies the estimate for the norm $\|B\|$ of B ,

$$\|B\| \leq C\|\beta\|_{L^\infty(\partial\Omega)}. \quad (19)$$

Now, we define a Born sequence u_n , $n \in \mathbb{Z}_+ := \mathbb{N} \cup \{0\}$ that satisfy

$$\begin{cases} \frac{d}{dt} u_0 + A_0 u_0 = F, \\ u_0|_{t=0} = 0, \end{cases} \quad (20)$$

$$\begin{cases} \frac{d}{dt} u_n + A_0 u_n = -B u_{n-1} + F, \\ u_n|_{t=0} = 0 \end{cases}$$

for $n \in \mathbb{N}$.

C. Convergence

In this subsection, we will prove the convergence of the Born sequence u_n , $n \in \mathbb{Z}_+$. To see this, define $v_n (n = 0, 1, 2, \dots)$ by

$$\begin{cases} v_n := u_n - u_{n-1} = -S_0 B v_{n-1}, & n = 1, 2, \dots, \\ v_0 = u_0. \end{cases} \quad (21)$$

Then, we have

$$\begin{aligned} \|v_n\|_{W((0,T))} &= \|S_0 B v_{n-1}\|_{W((0,T))} \\ &\leq C \|B v_{n-1}\|_{L^2((0,T); H^1(\Omega)^*)} \\ &\leq C \|B\| \|v_{n-1}\|_{W((0,T))} \\ &\leq C \|\beta\|_{L^\infty(\partial\Omega)} \|v_{n-1}\|_{W((0,T))}, \quad n = 1, 2, \dots \end{aligned}$$

with some general constants $C > 0$ which may be different line by line. Therefore, the Born series

$$u_0 + (u_1 - u_0) + (u_2 - u_1) + \dots + (u_{n+1} - u_n) + \dots,$$

and hence, the Born sequence u_n , $n = 0, 1, 2, \dots$ converges to a unique $u \in W(0, T)$ if $C\|\beta\|_{L^\infty(\partial\Omega)} < 1$. From (20) and the boundedness of the operators A_0, B , this implies

$$\begin{cases} \frac{d}{dt} u + A_0 u = -Bu + F, \\ u|_{t=0} = 0. \end{cases} \quad (22)$$

By $Au - A_0 u = Bu$ and the uniqueness of the weak solution to (8), u is the weak solution to (8).

In the rest of this section, by using the above arguments that we have given so far in this section, we will give the existence of Green function for (8) with $g = 0$ and Poisson kernel for (8) with $f = 0$, respectively. We also give the convergence of their associated Born sequences to the Schwartz kernels. The Green function and Poisson kernel are the Schwartz kernels⁹ of the operators mapping $S : L^2((0, T); H^1(\Omega)^*) \ni f \mapsto u \in L^2((0, T); H^1(\Omega))$ of (8) with $g = 0$ and $P : L^2((0, T); H^{-1/2}(\partial\Omega)) \ni g \mapsto u \in L^2((0, T); H^1(\Omega))$ of (8) with $f = 0$. We refer to S and P as the Green operator and Poisson operator for (8), respectively.

The Poisson operator P can be given as $\lim_{\epsilon \rightarrow +0} S^\epsilon$, where S^ϵ is the Green operator for (8) with homogeneous boundary condition and $f = g \otimes \delta_{\partial\Omega_\epsilon}$. Here, $\delta_{\partial\Omega_\epsilon}$ is the Dirac delta function supported on $\partial\Omega_\epsilon$ and $\partial\Omega_\epsilon$ is the boundary of $\Omega_\epsilon = \{x \in \Omega : \text{dist}(x, \partial\Omega) > \epsilon\}$ with the distance $\text{dist}(x, \partial\Omega)$ between x and $\partial\Omega$. More precisely, S^ϵ consists of $S^{\epsilon+}$ and $S^{\epsilon-}$ defined over Ω_ϵ and $\Omega \setminus \overline{\Omega_\epsilon}$ with the homogeneous boundary condition $(\gamma\partial_\nu + \beta)S^{\epsilon-} = 0$ over $\partial\Omega$ and the transmission boundary condition

$$S^{\epsilon+} - S^{\epsilon-} = 0, \quad \gamma(\partial_\nu S^{\epsilon+} - \partial_\nu S^{\epsilon-}) = I$$

over $\partial\Omega_\epsilon$ with the identity operator I on $L^2((0, T); H^{-1/2}(\partial\Omega_\epsilon))$ (although the situation is slightly different from here, it is essentially the same as in the work of Nakamura-Wang¹⁵). Also, $\lim_{\epsilon \rightarrow +0} S^\epsilon$ means that for every $g \in L^2((0, T); H^{-1/2}(\partial\Omega))$, $\lim_{\epsilon \rightarrow +0} S^\epsilon(g \otimes \delta_{\partial\Omega_\epsilon})$ exists in $L^2((0, T); H^1(\Omega))$. Hence, it is enough to consider the existence of the Green function and its Born approximation.

We first show that $S, (-S_0 B)^j S$, $j = 0, 1, 2, \dots$ have Schwartz kernels in the space of distribution $\mathcal{D}'(\Omega_T \times \Omega_T)$ defined in $\Omega_T \times \Omega_T$. By Theorem III.3, each of these is a continuous linear map from $L^2((0, T); H^1(\Omega)^*)$ to $L^2((0, T); H^1(\Omega))$. We refer to this as the L^2 -type continuity. Based on this, we will show that they have Schwartz kernels. Since the further arguments are the same for each of these maps, we only confine our argument to S . What we need to show is that $S : C_0^\infty(\Omega_T) \rightarrow \mathcal{D}'(\Omega_T)$ is linear and continuous, where $\mathcal{D}'(\Omega)$ is the space of distribution defined in Ω_T . We refer to this as the distribution-type continuity. Since the linearity of S is clear, we only need to show the continuity of S . In order to see this, let $\varphi_\ell \in C_0^\infty(\Omega_T)$, $\ell = 1, 2, \dots$ be a sequence such that $\text{supp } \varphi_\ell \subset K$, $\ell = 1, 2, \dots$ for a compact set $K \subset \Omega_T$ and for each $m \in \mathbb{Z}_+$, $\partial_{t,x}^\alpha \varphi_\ell$, $|\alpha| \leq m$ go to zero uniformly in Ω_T as $\ell \rightarrow \infty$, where $\partial_{t,x}^\alpha = \partial_t^{\alpha_0} \partial_{x_1}^{\alpha_1} \dots \partial_{x_3}^{\alpha_3}$, $\alpha = (\alpha_0, \alpha_1, \alpha_2, \alpha_3)$, $|\alpha| = \alpha_0 + \alpha_1 + \alpha_2 + \alpha_3$, $\text{supp } \varphi_\ell$ denotes the support of φ_ℓ , and $C_0^\infty(\Omega_T)$ is the set of all smooth functions with supports in Ω_T . We denote this as $\varphi_\ell \Rightarrow 0 (\ell \rightarrow \infty)$ and denote by $\mathcal{D}(\Omega_T)$ the topological vector space $C_0^\infty(\Omega_T)$ equipped with the topology induced by the convergence of sequence $\varphi_\ell \Rightarrow 0 (\ell \rightarrow \infty)$. Then, $\varphi_\ell \Rightarrow 0 (\ell \rightarrow \infty)$ implies $\varphi_\ell \rightarrow 0$, $\ell \rightarrow \infty$ in $L^2((0, T); H^1(\Omega)^*)$, and hence, we have that by the L^2 -type continuity of S , $S\varphi_\ell \rightarrow 0$, $\ell \rightarrow \infty$ in $L^2((0, T); H^1(\Omega))$. This immediately gives us the distribution-type continuity of S described as follows: for any fixed $\psi \in C_0^\infty(\Omega_T)$,

$$\langle S\varphi_\ell, \psi \rangle = \int_{\Omega_T} (S\varphi_\ell)(x, t) \psi(x, t) dx dt \rightarrow 0, \quad \ell \rightarrow \infty,$$

where $\langle S\varphi_\ell, \psi \rangle$ denotes the pairing between $S\varphi_\ell \in \mathcal{D}'(\Omega_T)$ and $\psi \in C_0^\infty(\Omega_T)$. Then, by the Schwartz kernel theorem, S has its unique Schwartz kernel $H(x, t; y, s) \in \mathcal{D}'(\Omega_T \times \Omega_T)$ such that

$$\langle S\varphi, \psi \rangle = \langle H(x, t; y, s), \psi(x, t) \otimes \varphi(y, s) \rangle, \quad \varphi(y, s), \psi(x, t) \in C_0^\infty(\Omega_T). \quad (23)$$

Now, recall (21) and the convergence of the Born sequence $u_n = T_n F$, $n = 0, 1, \dots$ with $T_n := \sum_{j=0}^n (-S_0 B)^j S F$, $n = 0, 1, \dots$, where we take F given by (12) with $g = 0$. Then, by (23) and the denseness of the finite linear combinations of the functions of the form $\psi(x, t) \otimes \varphi(y, s)$, $\varphi, \psi \in C_0^\infty(\Omega_T)$ in $\mathcal{D}(\Omega_T \times \Omega_T)$ which is defined similarly as $\mathcal{D}(\Omega_T)$, the sequence of Schwartz kernels $H_n^0(x, t; y, s) \in \mathcal{D}'(\Omega_T \times \Omega_T)$, $n = 0, 1, \dots$ of T_n , $n = 0, 1, \dots$ converges to $H(x, t; y, s) \in \mathcal{D}'(\Omega_T \times \Omega_T)$ as $n \rightarrow \infty$.

IV. BORN APPROXIMATION FOR POISSON KERNEL

Let us consider the following initial boundary value problem for u :

$$\begin{cases} (\partial_t - \gamma \Delta + b)u = 0, & (x, t) \in \Omega_T, \\ \gamma \partial_\nu u + \beta u = g, & (x, t) \in \partial\Omega_T, \\ u = 0, & x \in \Omega, \quad t = 0, \end{cases} \quad (24)$$

where Ω is either the half space $\Omega = \mathbb{R}_+^3 := \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_3 > 0\}$ or slab domain $\Omega = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : 0 < x_3 < L\}$. We assume that γ is a positive constant and b, β are nonnegative constants. Here, $g = g(x_1, x_2, t)$ is the boundary source.

We have already shown in Sec. III the existence of Poisson kernel and the convergence of the associated Born series. The aim of this section is to give an explicit form of the Poisson kernel when Ω is the aforementioned special and simple domains. The half space and slab domain have been used in DOT. For example, the slab geometry was used for fluorescent DOT¹⁶ and DOT for spatially modulated structured light was developed in the half space.¹³ In these studies, the time-independent diffusion equation was used.

A. Poisson kernel

Let us begin by considering u_0 satisfying the following diffusion equation:

$$\begin{cases} (\partial_t - \gamma \Delta + b)u_0 = 0, & (x, t) \in \Omega_T, \\ \gamma \partial_\nu u_0 = g, & (x, t) \in \partial\Omega_T, \\ u_0 = 0, & x \in \Omega, \quad t = 0. \end{cases} \quad (25)$$

If we have the Poisson kernel $G(x, t; y_1, y_2, s)$ for (25) which is the Schwartz kernel of the operator P_0 given in Definition III.4, then $u_0(x, t)$ can be given as

$$u_0(x, t) = \int_{\partial\Omega_T} G(x, t; y_1, y_2, s) g(y_1, y_2, s) dy_1 dy_2 ds.$$

Below, we calculate the Poisson kernel $G(x, t; y_1, y_2, s)$ in the half space and slab domain.

1. Half space

Let us consider the case of the half space, i.e., $\Omega = \mathbb{R}_+^3$ and $\partial\Omega = \mathbb{R}^2$. The Poisson kernel G satisfies

$$\begin{cases} (\partial_t - \gamma \Delta + b)G = 0, & (x, t) \in \Omega_T, \\ \gamma \partial_\nu G = \delta(x_1 - y_1)\delta(x_2 - y_2)\delta(t - s), & (x, t) \in \partial\Omega_T, \\ G = 0, & x \in \Omega, \quad t = 0. \end{cases} \quad (26)$$

Let us introduce $K(x, t; y, s)$ that satisfies

$$\begin{cases} (\partial_t - \gamma \Delta + b)K = \delta(x - y)\delta(t - s), & (x, t) \in \mathbb{R}^3 \times (0, T), \\ K = 0, & x \in \mathbb{R}^3, \quad t = 0. \end{cases}$$

We will obtain $K(s, t; y, s)$ by using its Laplace-Fourier transform,

$$\hat{K}(x_3, y_3) = \hat{K}(x_3; p, q; y, s) = \int_0^\infty \int_{\mathbb{R}^2} e^{-pt} e^{-i(q_1 x_1 + q_2 x_2)} K(x, t; y, s) dx_1 dx_2 dt.$$

Then, $\hat{K}$ has to satisfy

$$-\frac{d^2}{dx_3^2} \hat{K} + \lambda^2 \hat{K} = e^{-ps} e^{-i(q_1 y_1 + q_2 y_2)} \delta(x_3 - y_3), \quad x_3 \in \mathbb{R}^3,$$

with

$$\lambda = \sqrt{\frac{b+p}{\gamma} + q \cdot q}. \quad (27)$$

The above equation can be solved by the Fourier transform with respect to x_3 , and we obtain

$$\hat{K}(x_3, y_3) = \frac{1}{2\lambda\gamma} e^{-ps} e^{-i(q_1 y_1 + q_2 y_2)} e^{-\lambda|x_3 - y_3|}. \quad (28)$$

Thus, we have

$$K(x, t; y, s) = \theta(t-s) \frac{e^{-b(t-s)}}{[4\pi\gamma(t-s)]^{3/2}} e^{-\frac{(x-y)^2}{4\gamma(t-s)}}, \quad (29)$$

where $\theta(t)$ is the Heaviside step function, i.e., $\theta = 1$ for $t \geq 0$ and $\theta = 0$ for $t < 0$. Finally, from the argument in [Appendix B](#), we see $\hat{G} = 2\hat{K}$ and obtain

$$\begin{aligned} G(x, t; y_1, y_2, s) &= 2K(x, t; y, s) \\ &= \theta(t-s) \frac{2e^{-b(t-s)}}{[4\pi\gamma(t-s)]^{3/2}} e^{-\frac{(x_1 - y_1)^2 + (x_2 - y_2)^2 + x_3^2}{4\gamma(t-s)}}, \end{aligned} \quad (30)$$

where we put $y_3 = 0$.

2. Slab domain

In the case of the slab domain of width L , we set $\Omega = \{x \in \mathbb{R}^3; 0 < x_3 < L\}$. The Poisson kernel G satisfies

$$\begin{cases} (\partial_t - \gamma\Delta + b)G = 0, & (x, t) \in \Omega_T, \\ \gamma\partial_\nu G = \delta(x_1 - y_1)\delta(x_2 - y_2)\delta(t-s), & x_3 = 0, (x_1, x_2) \in \mathbb{R}^2, t \in (0, T), \\ \partial_\nu G = 0, & x_3 = L, (x_1, x_2) \in \mathbb{R}^2, t \in (0, T), \\ G = 0, & x \in \Omega, \quad t = 0. \end{cases}$$

Using an argument similar to [Appendix B](#), we can move the boundary source to the source term in the diffusion equation as $(\partial_t - \gamma\Delta + b)G = f(x_3)\delta(x_1 - y_1)\delta(x_2 - y_2)\delta(t-s)$ with the boundary condition $\partial_\nu G = 0$ at $x_3 = 0, L$, where $f(x_3) = \delta(x_3)$. Then, we can extend $f(x_3)$ as an even $2L$ -periodic function by setting $F(x_3) = f(x_3 - 2mL)$ for $2mL < x_3 \leq (2m+1)L$ and $F(x_3) = f(2(m+1)L - x_3)$ for $(2m+1)L \leq x_3 < 2(m+1)L$, where $m = 0, \pm 1, \pm 2, \dots$. We have

$$\begin{aligned} G(x, t; y_1, y_2, s) &= \int_{-\infty}^\infty K(x, t; y_1, y_2, \xi, s) F(\xi) d\xi \\ &= \sum_{m=-\infty}^\infty \left(\int_{2mL}^{(2m+1)L} + \int_{(2m+1)L}^{2(m+1)L} \right) K(x, t; y_1, y_2, \xi, s) F(\xi) d\xi \\ &= \sum_{m=-\infty}^\infty [K(x, t; y_1, y_2, 2mL, s) + K(x, t; y_1, y_2, 2(m+1)L, s)], \end{aligned}$$

where $K(x, t; y_1, y_2, \xi)$ is given by replacing x_3 by $x_3 - \xi$ in the previous $K(x, t; y, s)$ with $y_3 = 0$. Thus, in this case, we obtain

$$\begin{aligned} G(x, t; y_1, y_2, s) &= 2 \sum_{m=-\infty}^\infty K(x, t; y_1, y_2, 2mL, s) \\ &= \theta(t-s) \frac{2e^{-b(t-s)}}{[4\pi\gamma(t-s)]^{3/2}} e^{-\frac{(x_1 - y_1)^2 + (x_2 - y_2)^2}{4\gamma(t-s)}} \sum_{m=-\infty}^\infty e^{-\frac{(x_3 - 2mL)^2}{4\gamma(t-s)}}. \end{aligned}$$

B. Born sequence and Poisson kernel

Let us consider v_j ($j = 0, 1, \dots$) introduced in (21). The $(n + 1)$ th term v_n of the Born series satisfies

$$\begin{cases} (\partial_t - \gamma\Delta + b)v_n = 0, & (x, t) \in \Omega_T, \\ \gamma\partial_\nu v_n = -\beta v_{n-1}, & (x, t) \in \partial\Omega_T, \\ v_n = 0, & x \in \Omega, \quad t = 0, \end{cases}$$

for $n = 1, 2, \dots$. The initial term is given by $v_0 = u_0$. Using the Poisson kernel (30), we have

$$v_n(x, t) = -\beta \int_{\partial\Omega_T} G(x, t; y_1, y_2, s) v_{n-1}(y_1, y_2, 0, s) dy_1 dy_2 ds. \quad (31)$$

We then compute u as the limit of the Born sequence,

$$u = \lim_{n \rightarrow \infty} u_n, \quad u_n = v_0 + v_1 + \dots + v_n.$$

V. HALF SPACE CASE

In this section, we consider the diffusion equation (24) in the half space. That is, we take $\Omega = \mathbb{R}_+^3$ and $\partial\Omega = \mathbb{R}^2$. Let

$$g(x_1, x_2, t) = \delta(x_1)\delta(x_2)\delta(t - t_0), \quad t_0 > 0.$$

Then, by using the Poisson kernel (30), we have

$$\begin{aligned} v_0(x, t) &= G(x, t; 0, 0, t_0), \\ v_n(x, t) &= -2\beta \int_0^t \int_{\mathbb{R}^2} \frac{e^{-b(t-s)}}{[4\pi\gamma(t-s)]^{3/2}} e^{-\frac{(x_1-y_1)^2 + (x_2-y_2)^2 + x_3^2}{4\gamma(t-s)}} v_{n-1}(y_1, y_2, 0, s) dy_1 dy_2 ds. \end{aligned}$$

Let us introduce $w_n(x_3, t)$ ($n = 0, 1, 2, \dots$) as

$$v_n(x, t) = \frac{e^{-b(t-t_0)}}{t - t_0} e^{-\frac{x_1^2 + x_2^2}{4\gamma(t-t_0)}} w_n(x_3, t).$$

From the definition of G , we have

$$w_0(x_3, t) = \theta(t - t_0) \frac{1}{4(\pi\gamma)^{3/2} \sqrt{t - t_0}} e^{-\frac{x_3^2}{4\gamma(t-t_0)}}.$$

We have the following recurrence relation for w_n ($n \geq 1$):

$$w_n(x_3, t) = \frac{-\beta}{\sqrt{\pi\gamma}} \int_0^t \frac{w_{n-1}(0, s)}{\sqrt{t-s}} e^{-\frac{x_3^2}{4\gamma(t-s)}} ds. \quad (32)$$

Lemma V.1. From the recurrence relation (32), we can show that

$$\|w_n\|_{L^1((0, T); L^\infty((0, \infty)))} \leq \frac{\beta}{2} \sqrt{\frac{\pi T}{\gamma}} \|w_{n-1}\|_{L^1((0, T); L^\infty((0, \infty)))},$$

where $L^\infty((0, \infty))$ is the set of all bounded measurable function defined in $(0, \infty)$ and $L^1((0, T); L^\infty((0, \infty)))$ is the set of all $L^\infty((0, \infty))$ valued functions that are integrable over $(0, T)$ with respect to the norm of $L^\infty((0, \infty))$.

Proof. We note that

$$w_n(0, t) = \frac{-\beta}{\sqrt{\pi\gamma}} \int_0^t \frac{w_{n-1}(0, s)}{\sqrt{t-s}} ds.$$

This relation implies that if $w_{n-1}(0, s)$ does not change the sign, i.e., $w_{n-1}(0, s) \geq 0$ for all $s \in (0, T)$ or $w_{n-1}(0, s) \leq 0$ for all $s \in (0, T)$, then $w_n(0, t)$ does not change the sign neither on $(0, T)$. Indeed, we see by induction that the sign of $w_n(0, t)$ remains the same on $(0, T)$ for all $n = 0, 1, \dots$ since $w_0(0, t)$ is non-negative on $(0, T)$.

Keeping the above fact in mind, we have

$$|w_n(0, t)| = \frac{\beta}{\sqrt{\pi\gamma}} \left| \int_0^t \frac{w_{n-1}(0, s)}{\sqrt{t-s}} ds \right| = \frac{\beta}{\sqrt{\pi\gamma}} \int_0^t \frac{|w_{n-1}(0, s)|}{\sqrt{t-s}} ds.$$

Hence,

$$\begin{aligned} \int_0^T |w_n(0, t)| 2\sqrt{T-t} dt &= \frac{\beta}{\sqrt{\pi\gamma}} \int_0^T 2\sqrt{T-t} \int_0^t \frac{|w_{n-1}(0, s)|}{\sqrt{t-s}} ds dt \\ &= \frac{\beta}{\sqrt{\pi\gamma}} \int_0^T |w_{n-1}(0, s)| \int_s^T \frac{2\sqrt{T-t}}{\sqrt{t-s}} dt ds \\ &= \frac{\beta}{\sqrt{\pi\gamma}} \int_0^T |w_{n-1}(0, s)| \pi(T-s) ds \\ &\leq \frac{\beta\sqrt{T}}{\sqrt{\pi\gamma}} \int_0^T |w_{n-1}(0, s)| \pi\sqrt{T-s} ds. \end{aligned}$$

Noting that $2\sqrt{T-s} = \int_s^T (1/\sqrt{t-s}) dt$, we obtain

$$\int_0^T |w_n(0, s)| \int_s^T \frac{1}{\sqrt{t-s}} dt ds \leq \frac{\beta\sqrt{T}}{2} \sqrt{\frac{\pi}{\gamma}} \int_0^T |w_{n-1}(0, s)| \int_s^T \frac{1}{\sqrt{t-s}} dt ds.$$

The above integrals can be rewritten as

$$\int_0^T \int_0^t \frac{|w_n(0, s)|}{\sqrt{t-s}} ds dt \leq \frac{\beta\sqrt{T}}{2} \sqrt{\frac{\pi}{\gamma}} \int_0^T \int_0^t \frac{|w_{n-1}(0, s)|}{\sqrt{t-s}} ds dt.$$

Therefore,

$$\int_0^T \left| \int_0^t \frac{w_n(0, s)}{\sqrt{t-s}} ds \right| dt \leq \frac{\beta\sqrt{T}}{2} \sqrt{\frac{\pi}{\gamma}} \int_0^T \left| \int_0^t \frac{w_{n-1}(0, s)}{\sqrt{t-s}} ds \right| dt.$$

This means we have

$$\int_0^T \left\| \int_0^t \frac{w_n(0, s)}{\sqrt{t-s}} e^{-\frac{x_3^2}{4\gamma(t-s)}} ds \right\|_{L^\infty((0, \infty))} dt \leq \frac{\beta\sqrt{T}}{2} \sqrt{\frac{\pi}{\gamma}} \int_0^T \left\| \int_0^t \frac{w_{n-1}(0, s)}{\sqrt{t-s}} e^{-\frac{x_3^2}{4\gamma(t-s)}} ds \right\|_{L^\infty((0, \infty))} dt.$$

Thus, the proof is complete. □

Thus, the series $\sum_{n=0}^\infty w_n$ and $\sum_{n=0}^\infty u_n$ converge if

$$\beta < 2\sqrt{\frac{\gamma}{\pi T}}. \quad (33)$$

As we will see below from the explicit calculation of w_n , indeed, the series converges for any β (see Remark V.2).

Explicit expressions of $w_n(x_3, t)$ are available as follows. For $n \geq 1$, the functions $w_n(x_3, t)$ satisfy

$$\begin{aligned}
 w_n(x_3, t) &= \frac{(-\beta)^n}{4(\pi\gamma)^{(n+3)/2}} \int_{t_0}^t \int_{t_0}^{t_1} \cdots \int_{t_0}^{t_n} \frac{e^{-x_3^2/[4\gamma(t-t_n)]}}{\sqrt{(t-t_n)(t_n-t_{n-1}) \cdots (t_2-t_1)(t_1-t_0)}} dt_1 \cdots dt_n \\
 &= \frac{(-\beta)^n (t-t_0)^{(n-1)/2}}{4(\pi\gamma)^{(n+3)/2}} \left[\prod_{j=1}^{n-1} \int_0^1 \frac{s^{\frac{j}{2}-1}}{\sqrt{1-s}} ds \right] \int_0^1 \frac{s^{\frac{n}{2}-1}}{\sqrt{1-s}} e^{-x_3^2/[4\gamma(t-t_0)(1-s)]} ds \\
 &= \frac{(-\beta)^n (t-t_0)^{(n-1)/2}}{4(\pi\gamma)^{(n+3)/2}} \left[\prod_{j=1}^{n-1} B\left(\frac{j}{2}, \frac{1}{2}\right) \right] e^{-\zeta^2} \int_0^\infty e^{-\zeta^2 s} s^{\frac{n}{2}-1} (1+s)^{-\frac{n+1}{2}} ds \\
 &= \frac{(-\beta)^n (t-t_0)^{(n-1)/2}}{4(\pi\gamma)^{(n+3)/2}} \frac{2 \left\lfloor \frac{n-1}{2} \right\rfloor \pi \left\lfloor \frac{n}{2} \right\rfloor}{(n-2)!!} \\
 &\times \left[B\left(\frac{n}{2}, \frac{1}{2}\right) {}_1F_1\left(\frac{1-n}{2}, \frac{1}{2}; -\zeta^2\right) - 2\sqrt{\pi}\zeta {}_1F_1\left(1 - \frac{n}{2}, \frac{3}{2}; -\zeta^2\right) \right],
 \end{aligned} \tag{34}$$

where the floor function $\lfloor \cdot \rfloor$ is defined such that $\lfloor x \rfloor$ ($x \in \mathbb{R}$) denotes the largest integer that does not exceed x , and double factorials $n!! = n.(n-2).(n-4) \cdots$ are defined with $(-1)!! = 0!! = 1$. Here, $\zeta = x_3/\sqrt{4\gamma(t-t_0)}$, B is the beta function, and ${}_1F_1$ is the Kummer confluent hypergeometric function of the first kind. See [Appendix C](#) for the computation of $w_n(x_3, t)$. In particular, we have

$$w_n(0, t) = \frac{(-\beta)^n (t-t_0)^{(n-1)/2}}{4(\pi\gamma)^{(n+3)/2}} \frac{2 \left\lfloor \frac{n}{2} \right\rfloor \pi \left\lfloor \frac{n+1}{2} \right\rfloor}{(n-1)!!}.$$

Finally, we arrive at

$$\begin{aligned}
 u(x, t) &= v_0(x, t) + v_1(x, t) + \cdots \\
 &= \frac{e^{-b(t-t_0)}}{t-t_0} e^{-\frac{x_1^2+x_2^2}{4\gamma(t-t_0)}} [w_0(x_3, t) + w_1(x_3, t) + \cdots].
 \end{aligned} \tag{35}$$

Remark V.2. Due to the double factorial $(n-2)!!$ in the denominator of each n th term of $w_0 + w_1 + \cdots$ in (34), clearly $|w_n/w_{n-1}| < 1$ for sufficiently large n . Therefore, the series $\sum_{n=0}^\infty w_n$, and thus, $\sum_{n=0}^\infty v_n$ locally uniformly converge regardless of the value of β .

VI. NUMERICAL CALCULATION

For numerical calculation, we set t_0 to be zero [cf. (3)] and also set $x_1 = x_2 = 0$. Then, the n th Born approximation for (35) is written as

$$u_n(x_3, t) = \frac{e^{-bt}}{t} \sum_{j=0}^n w_j(x_3, t). \tag{36}$$

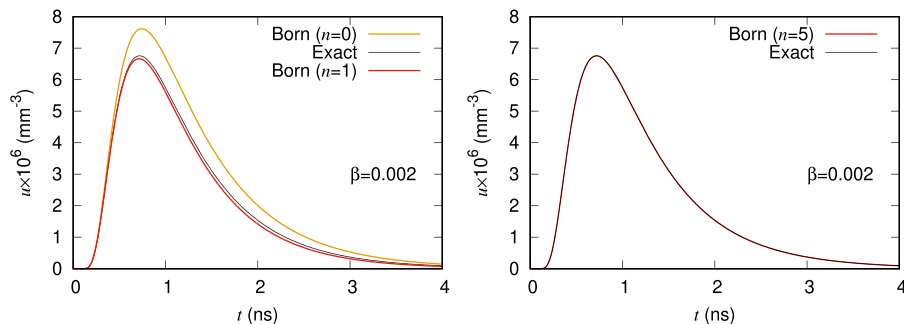


FIG. 2. The energy density u is plotted at $x_3 = 20$ mm as a function of t for $\beta = 0.002$ mm/ps. (Left) From the top, $u_0(x_3, t)$, $u_1(x_3, t)$, and $u_2(x_3, t)$ are shown. (Right) We plot $u_5(x_3, t)$ and $u(x_3, t)$. The two curves are almost identical.

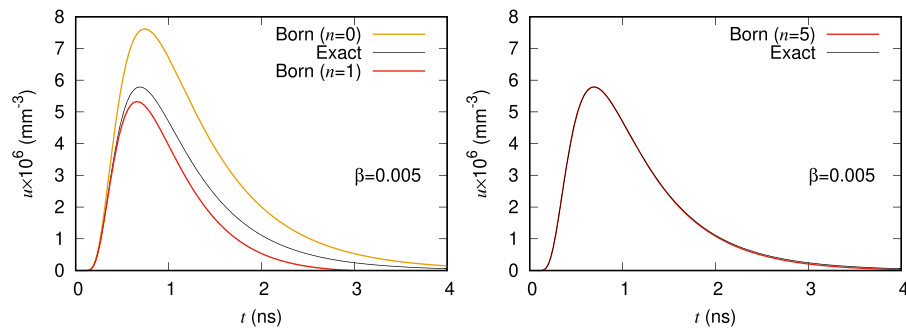


FIG. 3. The energy density u is plotted at $x_3 = 20$ mm as a function of t for $\beta = 0.005$ mm/ps. (Left) From the top, $u_0(x_3, t)$, $u(x_3, t)$, and $u_1(x_3, t)$ are shown. (Right) We plot $u_5(x_3, t)$ and $u(x_3, t)$. Two energy densities for $u(x_3, t)$ and $u_5(x_3, t)$ are almost indistinguishable.

Let us compare $u_n(x_3, t)$ in (36) and $u(x_3, t)$ in (4) using the parameter values given in (6). As is seen in Fig. 2, $n = 1$ is already a good approximation when $\beta = 0.002$. In Fig. 3, we set $\beta = 0.005$. We see that the energy density from the Born approximation of $n = 5$ becomes indistinguishable from the exact solution. In Figs. 4 and 5, we set $\beta = 0.015$. Since the value of β is larger, we need to take more terms. We arrive at the numerically exact result for $n = 70$.

The left panel of Fig. 5 suggests how the necessary number of terms n can be determined. Since results from different n agree for short time, we should use n such that curves for terms greater than or equal to n agree until $t = T$. Although it is not easy to know the optimal n *a priori*, we can find such n by trying several n 's.

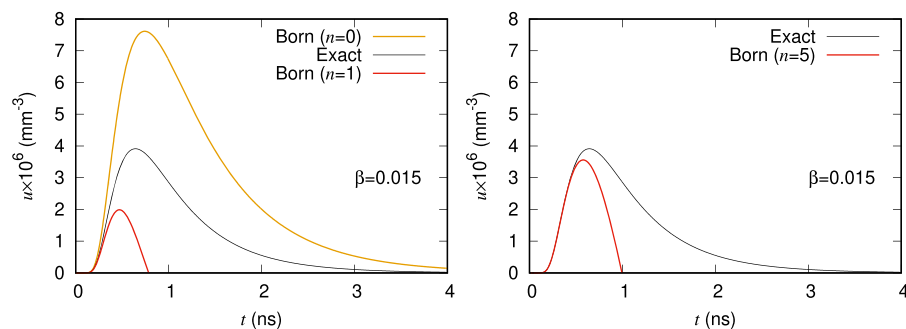


FIG. 4. The energy density u is plotted at $x_3 = 20$ mm as a function of t for $\beta = 0.015$ mm/ps. (Left) From the top, $u_0(x_3, t)$, $u(x_3, t)$, and $u_1(x_3, t)$ are shown. (Right) From the top, $u_5(x_3, t)$ and $u(x_3, t)$ are shown.

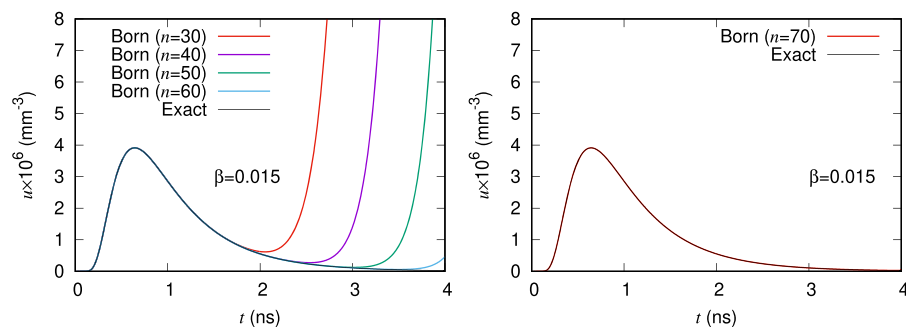


FIG. 5. Same as Fig. 4 but the 30th through 70th Born approximations are presented. (Left) From the top to the bottom, $u_{30}(x_3, t)$, $u_{40}(x_3, t)$, $u_{50}(x_3, t)$, $u_{60}(x_3, t)$, and $u(x_3, t)$ are shown. The curves show an excellent agreement except their tails. (Right) The results for $u_{70}(x_3, t)$ and $u(x_3, t)$ are shown. The case of $n = 70$ gives a numerically exact result.

Numerical calculation was done by Mathematica using a single Intel Core i5 (2.9 GHz). The computation time for $\beta = 0.002$, $n = 5$, in Fig. 2 and $\beta = 0.005$, $n = 5$, in Fig. 3 were 0.4 sec, whereas for $\beta = 0.015$ in Fig. 5, the cases $n = 30, 40, 50, 60, 70$ required 2.4, 3.3, 4.8, 6.0, and 7.7 s, respectively. The present formulation is beneficial when the Robin boundary condition with small β is considered. If we suppose that the diffusion approximation holds on the boundary and assume the diffuse surface reflection, we have $\beta = c/(2A)$, where c is the speed of light in the medium and $A = (1 + r_d)/(1 - r_d)$ with the internal reflection r_d .⁷ Let us suppose the reflective index outside the medium is unity. The refractive indices $n = 1.7, 2.3$, and 2.9 correspond to $\beta = 0.016, 0.0053$, and 0.0020 , respectively.

VII. CONCLUDING REMARKS

In Sec. VI, we considered the half space case and validated our approach of applying the Born series for boundary conditions. The comparison of Figs. 1 and 2 suggests that the present approach provides an efficient alternative formula for small β when the approximation with the extrapolated boundary condition does not work well. It is important for our formulation that the solution for the Neumann boundary condition has a simple explicit form. We explored the Poisson kernel in the half space and slab domain in Sec. IV. Applying the present strategy to other geometries is an interesting future problem.

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APPENDIX A: EXACT SOLUTIONS

Here, we compute the Poisson kernel for the three space dimensional half space, i.e., we solve (1). See also Refs. 8 and 23. Define

$$\phi := u - G$$

with G given in (26). Then, ϕ satisfies

$$\begin{cases} (\partial_t - \gamma \Delta + b)\phi = 0, & x \in \Omega, \quad t > 0, \\ \gamma \partial_\nu \phi + \beta \phi = -\beta G, & x \in \partial\Omega, \quad t > 0, \\ \phi = 0, & x \in \Omega, \quad t = 0. \end{cases}$$

Recall that λ is given in (27). The Laplace-Fourier transform given by

$$\hat{\phi}(x_3; p, q; y_1, y_2, s) = \int_0^\infty \int_{\mathbb{R}^2} e^{-pt} e^{-i(q_1 x_1 + q_2 x_2)} \phi(x, t; y_1, y_2, s) dx_1 dx_2 dt$$

satisfies

$$\begin{cases} -\frac{d^2}{dx_3^2} \hat{\phi} + \lambda^2 \hat{\phi} = 0, & x_3 > 0, \\ -\gamma \frac{d\hat{\phi}}{dx_3} + \beta \hat{\phi} = -\beta \hat{G}, & x_3 = 0. \end{cases}$$

On the other hand, we have (28) and $\hat{G}$ can be given by

$$\hat{G}(x_3; p, q; y_1, y_2, s) = \frac{1}{\lambda \gamma} e^{-ps - i(q_1 y_1 + q_2 y_2)} e^{-\lambda x_3}. \quad (\text{A1})$$

Here, we used the relation $\hat{G} = 2\hat{K}$ (see Appendix B). Hence,

$$\hat{\phi}(x_3) = \frac{-\beta}{\beta + \lambda\gamma} \hat{G}(0) e^{-\lambda x_3} = \frac{-\beta}{\lambda\gamma(\beta + \lambda\gamma)} e^{-ps} e^{-i(q_1 y_1 + q_2 y_2)} e^{-\lambda x_3}. \quad (\text{A2})$$

Furthermore, from the relation

$$\frac{d}{dx_3} \hat{\phi}(x_3) = \frac{2\beta}{\gamma} \hat{K}(x_3, 0) + \frac{\beta}{\gamma} \hat{\phi}(x_3)$$

which can be readily verified using (28) and (A2), we have

$$\hat{\phi}(x_3) = -\frac{2\beta}{\gamma} \int_{x_3}^{\infty} e^{\frac{\beta}{\gamma}(x_3 - \xi)} \hat{K}(\xi, 0) d\xi.$$

Thus, we arrive at the following solution:

$$\begin{aligned} u(x, t) &= G(x, t; y_1, y_2, t_0) - \frac{2\beta}{\gamma} \int_{x_3}^{\infty} e^{\frac{\beta}{\gamma}(x_3 - \xi)} K(x_1, x_2, \xi, t; y_1, y_2, 0, t_0) d\xi \\ &= \theta(t - t_0) \frac{2e^{-b(t-t_0)}}{[4\pi\gamma(t-t_0)]^{3/2}} e^{-\frac{(x_1-y_1)^2 + (x_2-y_2)^2 + x_3^2}{4\gamma(t-t_0)}} \\ &\quad - \theta(t - t_0) \frac{\beta e^{-b(t-t_0)}}{4\pi\gamma^2(t-t_0)} e^{-\frac{(x_1-y_1)^2 + (x_2-y_2)^2}{4\gamma(t-t_0)}} e^{\frac{\beta}{\gamma}(x_3 + \beta(t-t_0))} \operatorname{erfc}\left(\frac{x_3 + 2\beta(t-t_0)}{\sqrt{4\gamma(t-t_0)}}\right), \end{aligned}$$

where G is given in (30).

APPENDIX B: AN INTERPRETATION OF TRANSIENT BOUNDARY POINT SOURCE

By using the advantage of the simple geometry for Ω , we will explain more explicitly than given before in Sec. III how the solution u of (1) with a transient boundary point source can be obtained as a limit of the solution u_ϵ of the following initial boundary value problem with a transient point source:

$$\begin{cases} (\partial_t - \gamma\Delta + b)u_\epsilon = g\delta(x_3 - \epsilon), & (x, t) \in \Omega_T, \\ \gamma\partial_\nu u_\epsilon + \beta u_\epsilon = 0, & (x, t) \in \partial\Omega_T, \\ u_\epsilon = 0, & x \in \Omega, \quad t = 0 \end{cases}$$

with $g = \delta(x_1 - y_1)\delta(x_2 - y_2)\delta(t - s)$. We prepare the following G_ϵ :

$$\begin{cases} (\partial_t - \gamma\Delta + b)G_\epsilon = g\delta(x_3 - \epsilon), & (x, t) \in \Omega_T, \\ \gamma\partial_\nu G_\epsilon = 0, & (x, t) \in \partial\Omega_T, \\ G_\epsilon = 0, & x \in \Omega, \quad t = 0 \end{cases}$$

with the same g as above. Similar to the calculation in Appendix A, let us consider u_ϵ in the form

$$\phi_\epsilon = u_\epsilon - G_\epsilon. \quad (\text{B1})$$

Here, ϕ_ϵ satisfies

$$\begin{cases} (\partial_t - \gamma\Delta + b)\phi_\epsilon = 0, & (x, t) \in \Omega_T, \\ \gamma\partial_\nu \phi_\epsilon + \beta\phi_\epsilon = -\beta G_\epsilon, & (x, t) \in \partial\Omega_T, \\ \phi_\epsilon = 0, & x \in \Omega, \quad t = 0. \end{cases}$$

We obtain

$$\hat{\phi}_\epsilon(x_3) = \frac{-\beta}{\beta + \lambda\gamma} \hat{G}_\epsilon(0) e^{-\lambda x_3}.$$

Here,

$$\hat{G}_\epsilon(x_3) = \int_0^\infty \int_{\mathbb{R}^2} e^{-pt} e^{-i(q_1 x_1 + q_2 x_2)} G_\epsilon(x, t; y_1, y_2, \epsilon, s) dx_1 dx_2 dt.$$

We note that

$$G_\epsilon(x, t; y_1, y_2, \epsilon, s) = K(x, t; y_1, y_2, \epsilon, s) + K(x, t; y_1, y_2, -\epsilon, s),$$

where K is given in (29). Therefore, we obtain

$$\hat{G}_\epsilon(x_3) = \frac{1}{2\lambda\gamma} e^{-ps} e^{-i(q_1 y_1 + q_2 y_2)} \left(e^{-\lambda|x_3 - \epsilon|} + e^{-\lambda|x_3 + \epsilon|} \right),$$

where we used (28). In the limit, we have $\lim_{\epsilon \rightarrow 0} \hat{G}_\epsilon = \hat{G}$, which is given in (A1). Thus, we arrive at

$$\hat{\phi}_\epsilon(x_3) = \frac{-\beta}{\lambda\gamma(\beta + \lambda\gamma)} e^{-ps} e^{-i(q_1 y_1 + q_2 y_2)} e^{-\lambda(x_3 + \epsilon)}.$$

We see that $\lim_{\epsilon \rightarrow 0} \hat{\phi}_\epsilon = \hat{\phi}$, which is given in (A2). Thus, we can directly see that the distribution u_ϵ converges to the distribution u as $\epsilon \rightarrow 0$.

APPENDIX C: SPECIAL FUNCTIONS

By using the formulae

$$B\left(a, \frac{1}{2}\right) B\left(a + \frac{1}{2}, \frac{1}{2}\right) = \frac{\pi}{a}, \quad B\left(\frac{1}{2}, \frac{1}{2}\right) = \pi,$$

we have

$$B\left(\frac{1}{2}, \frac{1}{2}\right) B\left(1, \frac{1}{2}\right) B\left(\frac{3}{2}, \frac{1}{2}\right) \cdots B\left(\frac{n-1}{2}, \frac{1}{2}\right) = \begin{cases} \frac{2^{\frac{n}{2}-1} \pi^{\frac{n}{2}}}{(n-2)!!} & (n \text{ even}), \\ \frac{2^{\frac{n-1}{2}} \pi^{\frac{n-1}{2}}}{(n-2)!!} & (n \text{ odd}). \end{cases}$$

Moreover,

$$B\left(\frac{n}{2}, \frac{1}{2}\right) = \frac{\Gamma\left(\frac{n}{2}\right) \Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{n+1}{2}\right)},$$

where $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$.

Now, recall that the Kummer confluent hypergeometric function of the first kind is given by

$${}_1F_1(a, b; z) = M(a, b; z) = \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n n!} z^n = 1 + \frac{a}{b} z + \frac{a(a+1)}{b(b+1)2!} z^2 + \cdots.$$

Then, we have

$$\begin{aligned} {}_1F_1\left(0, \frac{1}{2}; -z\right) &= 1, \\ {}_1F_1\left(-\frac{1}{2}, \frac{1}{2}; -z\right) &= e^{-z} + \sqrt{\pi z} \operatorname{erf}(\sqrt{z}), \\ {}_1F_1\left(-1, \frac{1}{2}; -z\right) &= 1 + 2z, \\ {}_1F_1\left(-\frac{3}{2}, \frac{1}{2}; -z\right) &= (1+z)e^{-z} + \sqrt{\pi z} \left(z + \frac{3}{2}\right) \operatorname{erf}(\sqrt{z}) \end{aligned}$$

and

$$\begin{aligned}
{}_1F_1\left(\frac{1}{2}, \frac{3}{2}; -z\right) &= \frac{1}{2} \sqrt{\frac{\pi}{z}} \operatorname{erf}(\sqrt{z}), \\
{}_1F_1\left(0, \frac{3}{2}; -z\right) &= 1, \\
{}_1F_1\left(-\frac{1}{2}, \frac{3}{2}; -z\right) &= \frac{e^{-z}}{2} + \frac{\sqrt{\pi z}}{2} \left(1 + \frac{1}{2z}\right) \operatorname{erf}(\sqrt{z}), \\
{}_1F_1\left(-1, \frac{3}{2}; -z\right) &= 1 + \frac{2}{3}z,
\end{aligned}$$

where

$$\operatorname{erf}(\sqrt{z}) = \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{z}} e^{-t^2} dt.$$

We close this appendix by giving some miscellaneous facts on hypergeometric function and error function that are useful for computing the Poisson kernel numerically. Besides the hypergeometric function given above explicitly, other hypergeometric functions can be recursively computed using the following recurrence relation:

$${}_1F_1(a-1, b; z) = \frac{2a-b+z}{a-b} {}_1F_1(a, b; z) - \frac{a}{a-b} {}_1F_1(a+1, b; z).$$

The following form is convenient to numerically evaluate the error function:

$$\operatorname{erf}(\xi) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n \xi^{2n+1}}{n!(2n+1)} = \frac{2}{\sqrt{\pi}} e^{-\xi^2} \sum_{n=0}^{\infty} \frac{2^n \xi^{2n+1}}{(2n+1)!!}.$$

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