EMERGENCE OF BOUNDARY CONDITION IN THE HEAT EQUATION

JAYWAN CHUNG, SEUNGMIN KANG, HO-YOUN KIM, AND YONG-JUNG KIM

Abstract. The Dirichlet and Neumann conditions are commonly employed as boundary conditions for the heat equation, yet their legitimacy is debatable in certain scenarios. This paper aims to demonstrate that, in fact, diffusion laws autonomously select boundary conditions. To illustrate this, we incorporate the bounded domain into a larger domain with a diffusivity parameter $\epsilon > 0$ and examine the solution's behavior at the interface. Our findings reveal that homogeneous Neumann or Dirichlet boundary conditions emerge as $\epsilon \to 0$, contingent upon the type of the heterogeneous diffusion.

1. Emerging boundary condition

An initial value problem of the heat equation in a bounded domain $\Omega_1 \subset \mathbb{R}^n$ can be written as

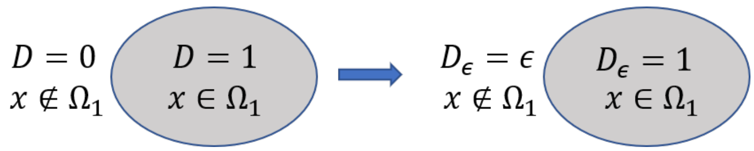
$$\begin{cases} U_t = \Delta U, & x \in \Omega_1, t > 0, \\ U = \phi(x), & x \in \Omega_1, t = 0, \end{cases} \tag{1.1}$$

where $U(t,x)$ is the density, U_t is the partial derivative with respect to the time variable t, $\Delta U = \sum_{i=1}^n \frac{\partial^2}{\partial x_i^2} U$ is the Laplacian of U, and $\phi \in L^\infty(\mathbb{R}^+)$ is an initial value. The composition of the problem is complete only after an appropriate boundary condition is provided on the boundary $\partial\Omega_1$. Among the various boundary conditions, Dirichlet and Neumann conditions are the most commonly used, which are, respectively,

$$\begin{cases} U = 0 \quad \text{for} \quad x \in \partial\Omega_1, t > 0, & \text{Dirichlet B.C.} \\ \dfrac{\partial U}{\partial \mathbf{n}} = 0 \quad \text{for} \quad x \in \partial\Omega_1, t > 0, & \text{Neumann B.C.} \end{cases} \tag{1.2}$$

where $\frac{\partial U}{\partial \mathbf{n}}$ is the directional derivative in the normal direction on the boundary. The physical meaning of boundary conditions is understood well, and it is "people" that choose a boundary condition as they deem appropriate. However, the freedom of choosing boundary conditions often causes the legitimacy to be disputed.

Rather than choosing a boundary condition, we can take the boundary condition that "appears" when domain Ω_1 is embedded in a larger domain, where the outside of Ω_1 is of diffusivity $D = 0$. Since there is no diffusion outside of Ω_1, the domain is essentially isolated from the outside, and the



solution behavior on the boundary $\partial\Omega_1$ is the boundary condition selected by the diffusion itself. There are two critical issues in this approach. First, the diffusion theory cannot handle the outer region with $D = 0$ directly. To handle this, we take a perturbed diffusivity,

$$D_\epsilon(x) = \begin{cases} \epsilon & \text{if } x \notin \Omega_1, \\ 1 & \text{if } x \in \Omega_1, \end{cases} \tag{1.3}$$

and consider the limit of the solution as $\epsilon \to 0$. The behavior of the limit along the boundary of the domain Ω_1 is what we need to find out.

The second issue is which diffusion equation to be chosen as a heterogeneous diffusion. There is no correct diffusion law agreed upon by everyone when the diffusivity $D_\epsilon = D_\epsilon(x)$ depends on the space variable. One of the most general ways to write a diffusion equation is

$$u_t = \nabla \cdot (K\nabla(Mu)), \quad D_\epsilon = KM. \tag{1.4}$$

The most popular case is $(K, M) = (D_\epsilon, 1)$, which is called Fick's diffusion law[3]. The case $(K, M) = (1, D_\epsilon)$ is also often used and is called Fokker-Plank or Chapman's diffusion law[1], which is related to the Ito stochastic integral. The case $(K, M) = (\sqrt{D_\epsilon}, \sqrt{D_\epsilon})$ is called Wereide's diffusion law [14] and is related to the Stratonovich stochastic integral. We consider a diffusion law in a general form,

$$u_t = \nabla \cdot (D_\epsilon^{1-q}\nabla(D_\epsilon^q u)), \quad q \in \mathbb{R}. \tag{1.5}$$

Then, the above three cases are respectively $q = 0, 1$, and 0.5. If $q \neq 0$, we may split the diffusion into Fick's law diffusion and an advection term, i.e.,

$$u_t = \nabla \cdot (D_\epsilon \nabla u) + \nabla \cdot (qu\nabla D_\epsilon). \tag{1.6}$$

The second term is the drift term. Because of this drift term, all cases where $q \neq 0$ can be called Fokker-Planck diffusion, not just the case where $q = 1$.

If we take the limit as $\epsilon \to 0$, the diffusivity disappears in the outer region, and the solution will converge to a solution of (1.1) in the region $x \in \Omega_1$. Hence, if we provide the boundary condition satisfied by the limit, it will give the same solution in the domain Ω_1. Hence, in this formulation of the problem, the only thing we care about is the emerging boundary condition of the limit of solutions of (1.5) as $\epsilon \to 0$, which may depend on the exponent $q \in \mathbb{R}$ and the dimension of the domain $\Omega_1 \subset \mathbb{R}^n$. It is proved in [4] that the homogeneous Neumann boundary condition emerges for the $q = 0$ case, which is the Fickian diffusion. However, for $q \neq 0$, we do not have an answer for general dimensions $n > 1$. For the dimension $n = 1$, we have a complete answer for all $q \in \mathbb{R}$, which is the result presented in the paper.

There have been lots of debates and discussions on the correct diffusion equation in heterogeneous environments. The two cases with $q = 0$ and $q = 1$ are mostly compared (see [10, 11]). These long-standing controversies were about finding the correct diffusion law among various diffusion laws. Landsberg and Sattin [12] said what matters is adding an appropriate drift term, not a diffusion law itself. However, the important thing is to know their connection as in (1.6). Kampen [5] clarified similar debates related to stochastic differential equations for probability density functions. Kampen [6] and Schnitzer [13] claimed that there is no universal form of the diffusion equation, but each system should be studied individually. In other words, the corresponding q may be different for each situation. If there is no such a constant q, (1.4) may serve as a more general diffusion equation.

2. One dimensional problem and Results

One-dimensional problem is often considered since it gives the essential physics of diffusion phenomena most clearly. Indeed, we can find the solution explicitly in a one-dimensional case and see the phenomenon in great detail, which is the purpose of the paper. We consider the case that $\Omega_1 = \{x > 0\}$ and hence, the boundary is the single point $x = 0$. Then, the problem (1.1) is written as

$$\begin{cases} U_t = U_{xx}, & t > 0,\ x > 0, \\ U = \phi(x), & t = 0,\ x > 0, \end{cases} \tag{2.1}$$

and the perturbed problem in the whole real line using the diffusion model (1.5) is written as

$$\begin{cases} u_t = (D_\epsilon^{1-q}(D_\epsilon^q u)_x)_x, & t > 0,\ x \in \mathbb{R}, \\ u(0, x) = \phi(x), & x \in \mathbb{R}, \end{cases} \tag{2.2}$$

where $\phi \in L^\infty(\mathbb{R})$, $q \in \mathbb{R}$, and D_ϵ is given by (1.3). Since the diffusivity D_ϵ is discontinuous at $x = 0$, the solution of (2.2) is not defined as a usual weak solution. For notational convenience, the domain with the interface $x = 0$ removed is denoted as

$$\Omega_b := \mathbb{R} \setminus \{0\} = \mathbb{R}^- \cup \mathbb{R}^+.$$

The solution of (2.2) in this paper is defined as follows, ensuring physical relevance. [1]

Definition 2.1. *A function $u \in C^{1,0}(\mathbb{R}^+ \times \Omega_b) \cap L^\infty(\mathbb{R}^+ \times \mathbb{R})$ is called a solution of* (2.2) *if the followings hold:*

[1]Another way to define the solution of (2.2) is in a weak sense. However, since the diffusivity D_ϵ is discontinuous at $x = 0$, the regularity should be given to the product $D_\epsilon^q u$. If $q = 0$, the regularity is given to u. If $q = 1$, we can define the solution in a very weak sense.

(*i*) *The function* u *satisfies additional regularities*

$$D_\epsilon^q u \in C^{0,1}(\mathbb{R}^+ \times \Omega_b) \cap C(\mathbb{R}^+ \times \mathbb{R}), \tag{2.3}$$

$$D_\epsilon^{1-q}(D_\epsilon^q u)_x \in C^{0,1}(\mathbb{R}^+ \times \Omega_b) \cap C(\mathbb{R}^+ \times \mathbb{R}). \tag{2.4}$$

(*ii*) *Eq.* (2.2) *is satisfied in the classical sense for all* $(t,x) \in \mathbb{R}^+ \times \Omega_b$.

(*iii*) *The initial condition is satisfied pointwise except at the interface, i.e.,*

$$\lim_{t\to 0^+} u(t,x) = \phi(x), \quad x \in \Omega_b.$$

We call $D_\epsilon^q u$ the *potential* and $D_\epsilon^{1-q}(D_\epsilon^q u)_x$ the *flux*. Note that the two regularity conditions, (2.3) and (2.4), are not given to the solution but to the potential and the flux. Furthermore, if $q \neq 1$, $D_\epsilon^q u$ has no chance to belong to $C^{0,1}(\mathbb{R}^+ \times \mathbb{R})$ since $D_\epsilon^{1-q}(D_\epsilon^q u)_x \in C(\mathbb{R}^+ \times \mathbb{R})$ and D_ϵ^{1-q} is discontinuous at $x = 0$. The main results of the paper are in the following theorem.

Theorem 2.1 (Boundary condition and regularity)**.** *Let* $\phi \in C(\Omega_b) \cap L^\infty(\mathbb{R})$ *with existing limits* $\phi(0^+)$ *and* $\phi(0^-)$, *satisfying* $\phi \geq 0$, $q \in \mathbb{R}$, *and* D_ϵ *be given by* (1.3). *Then the solution of* (2.2) *exists and is unique. The solution satisfies*

$$D_\epsilon^q u_t \in C(\mathbb{R}^+ \times \mathbb{R}) \quad \text{and} \quad D_\epsilon^q (D_\epsilon^{1-q}(D_\epsilon^q u)_x)_x \in C(\mathbb{R}^+ \times \mathbb{R}). \tag{2.5}$$

The solution $u(t,x;\epsilon)$ *converges pointwise for all* $x > 0$ *as* $\epsilon \to 0$, *and the limit, denoted by* $U(t,x)$, *satisfies* (2.1) *and a boundary condition,*

$$\begin{cases} U_x(t,0^+) = 0, & \text{if } q < 0.5, \\ U(t,0^+) = 0, & \text{if } q > 0.5. \end{cases} \tag{2.6}$$

Furthermore, as $\epsilon \to 0$,

$$\begin{cases} \big|u_x(t,0^+;\epsilon)\big| = O(\epsilon^{0.5-q}) & \text{if } q < 0.5, \\ |u(t,0^+;\epsilon)| = O(\epsilon^{q-0.5}) & \text{if } q > 0.5. \end{cases} \tag{2.7}$$

According to the theorem, the Neumann boundary condition emerges if $q < 0.5$. Therefore, if Fick's diffusion is taken, the zero-flux condition is a natural boundary condition. On the other hand, if $q > 0.5$, the Dirichlet boundary condition is the natural one. If it is the border case that $q = 0.5$, there is no restriction on the boundary condition. Equations (2.3) and (2.5) point out that if $q \neq 0$, the solution u, its time derivative u_t, and the spatial derivative of the flux $(D_\epsilon^{1-q}(D_\epsilon^q u)_x)_x$ have the same jump discontinuity at the interface $x = 0$ which become continuous after multiplying by D_ϵ^q. If we rewrite the equation (2.2) in terms of the pressure, $p = D_\epsilon^q u$, we obtain (3.2), and the pressure becomes a classical solution of it. We may extend the question to the multidimensional case with or without a reaction function. In fact, Hilhorst *et al.* [4] showed that the Neumann boundary condition emerges along the boundary of a bounded domain $\Omega \subset \mathbb{R}^n$ if Fick's diffusion law is taken with bistable nonlinearity.

The paper consists as follows. In Section 3, Theorem 2.1 is proved. We find the explicit formula of the solution and then prove the claims in the theorem one by one using the explicit formula. In Section 4, two examples of explicit solutions of (2.2) are given. These explicit solutions are useful to see the dynamics of the problem. In Section 5, we numerically test the convergence of boundary conditions as $\epsilon \to 0$. These numerical computations show us detailed convergence order of the boundary conditions as $\epsilon \to 0$, which are given in (2.7). In Section 6, we discuss why the boundary condition in (2.6) splits at $q = 0.5$. We consider the relationship between the diffusion equation (2.2) and the microscopic-scale random walk model. The case $q = 0.5$ corresponds to the one with a constant sojourn time. The heterogeneity in the sojourn time decides the boundary condition.

3. Proof of Main Results

This section is for the proof of Theorem 2.1. We first solve the problem explicitly and prove the theorem one by one which are divided into several lemmas. We reduce (2.2) to Fick's diffusion law by scaling the space variable and writing it in terms of the potential. First, introduce a new space variable

$$y := \int_0^x D_\epsilon^{-q}(s)\, ds, \tag{3.1}$$

and write the potential as

$$p(t,y) := D_\epsilon^q(x)u(t,x), \quad p_0(y) := D_\epsilon^q(x)\phi(x).$$

Since D_ϵ is constant respectively for $x < 0$ and $x > 0$, we have $D_\epsilon(y) = D_\epsilon(x)$ under the relation (3.1). Then,

$$p_t(t,y) = D_\epsilon^q u_t(t,x), \quad p_y(t,y) = D_\epsilon^q (D_\epsilon^q u(t,x))_x.$$

Therefore, in terms of the new variables, the flux is written as

$$D_\epsilon^{1-q}(D_\epsilon^q u)_x = D_\epsilon^{1-2q}(D_\epsilon^q u)_y = D_\epsilon^{1-2q} p_y = \begin{cases} \sigma p_y, & y < 0, \\ \ \ p_y, & y > 0, \end{cases}$$

where we denote $\sigma := \epsilon^{1-2q}$ for simplicity. Finally, the main equation (2.2) is written as

$$\begin{cases} p_t = (D_\epsilon^{1-2q} p_y)_y, & t > 0,\ y \in \mathbb{R}, \\ p(0,y) = p_0(y), & y \in \mathbb{R}. \end{cases} \tag{3.2}$$

The strategy to prove Theorem 2.1 is to solve (3.2) explicitly and prove the claims in the theorem using the explicit formula. Explicit solutions such as Gaussian, heat kernel, and Barenblatt solution have provided essential information about a general solution. The explicit solutions obtained in the paper play a similar role.

We define a solution of Problem (3.2) in a manner equivalent to Definition 2.1 as follows.

Definition 3.1. *A function $p \in C^{1,1}(\mathbb{R}^+ \times \Omega_b) \cap C(\mathbb{R}^+ \times \mathbb{R}) \cap L^\infty(\mathbb{R}^+ \times \mathbb{R})$ is called a solution of* (3.2) *if the followings hold:*

(*i*) *The function p satisfies an additional regularity*

$$D_\epsilon^{1-2q} p_y \in C^{0,1}(\mathbb{R}^+ \times \Omega_b) \cap C(\mathbb{R}^+ \times \mathbb{R}). \tag{3.3}$$

(*ii*) *Eq.* (3.2) *is satisfied in the classical sense for all* $(t,y) \in \mathbb{R}^+ \times \Omega_b$*.*

(*iii*) *The initial condition is satisfied pointwise except at the interface, i.e.,*

$$\lim_{t\to 0^+} p(t,y) = p_0(y), \quad y \in \Omega_b.$$

First, we establish the uniqueness of a solution in the sense of Definition 3.1.

Lemma 3.1. *There exists at most one solution of Problem* (3.2)*.*

Proof. It is sufficient to prove that the following problem (3.4) admits only the trivial solution.

$$\begin{cases} p_t = (D_\epsilon^{1-2q} p_y)_y, & t > 0,\ y \in \mathbb{R}, \\ p(0,y) = 0, & y \in \Omega_b. \end{cases} \tag{3.4}$$

The proof follows a method outlined in [15], $p.29 - 30$. For arbitrary $t_0 \in \mathbb{R}^+$ and $y_0 \in \Omega_b$, we define $\Psi(t,y) := \Phi(t_0 - t, y)$ for $(t,y) \in [0,t_0) \times \mathbb{R}$, where Φ is the fundamental solution of the equation

$$\begin{cases} \Phi_t = (D_\epsilon^{1-2q} \Phi_y)_y, & t > 0, y \in \mathbb{R}, \\ \Phi(0,y) = \delta(y - y_0), & y \in \mathbb{R}. \end{cases}$$

It is worth noting that the fundamental solution Φ can be explicitly expressed by employing $p(t,y) = p(t,y;\sigma)$ in (4.1) as:

$$\Phi(t,y) = \begin{cases} p(t,y;\sigma), & \text{if } y_0 > 0, \\ \frac{1}{\sqrt{\sigma}} p(t, -\frac{y}{\sqrt{\sigma}}; \frac{1}{\sqrt{\sigma}}), & \text{if } y_0 < 0. \end{cases}$$

For arbitrary large $R > |y_0|$, there exists $\varphi \in C^2(\mathbb{R})$ such that $0 \le \varphi(y) \le 1$ and satisfies

$$\varphi(y) = \begin{cases} 1, & \text{if } y \in (-R, R), \\ 0, & \text{if } y \in (-\infty, -R-1) \cup (R+1, \infty), \end{cases}$$

$|\varphi_y|,\ |\varphi_{yy}| \le C$, where C is a constant independent of R. For any solution $\tilde{p}$ of (3.4), we have

$$\begin{aligned} (\tilde{p}\varphi\Psi)_t &= \tilde{p}_t\varphi\Psi + \tilde{p}\varphi_t\Psi + \tilde{p}\varphi\Psi_t \\ &= (D_\epsilon^{1-2q}\tilde{p}_y)_y\varphi\Psi - (D_\epsilon^{1-2q}\Psi_y)_y\tilde{p}\varphi, \end{aligned} \tag{3.5}$$

for all $(t,y) \in (0,t_0) \times \Omega_b$. We integrate (3.5) over $(0,t_0) \times \mathbb{R}$. Then the integration of the left hand side is

$$\begin{aligned} \int_0^{t_0} \int_{\mathbb{R}} (\tilde{p}\varphi\Psi)_t dydt &= \lim_{t\to t_0} \int_{\mathbb{R}} \tilde{p}(t,y)\varphi(y)\Psi(t,y)dy \\ &= \tilde{p}(t_0, y_0). \end{aligned}$$

The integration of the right hand side is

$$\begin{aligned}
&\int_0^{t_0}\int_{\mathbb{R}^+}\tilde{p}_{yy}\varphi\Psi dydt+\int_0^{t_0}\int_{\mathbb{R}^-}\sigma\tilde{p}_{yy}\varphi\Psi dydt-\int_0^{t_0}\int_{\Omega_b}(D_\epsilon^{1-2q}\Psi_y)_y\tilde{p}\varphi dydt\\
&=-\int_0^{t_0}\int_{\mathbb{R}^+}\tilde{p}_y(\varphi\Psi)_y dydt-\int_0^{t_0}\int_{\mathbb{R}^-}\sigma\tilde{p}_y(\varphi\Psi)_y dydt-\int_0^{t_0}\int_{\Omega_b}(D_\epsilon^{1-2q}\Psi_y)_y\tilde{p}\varphi dydt\\
&=\int_0^{t_0}\int_{\mathbb{R}^+}\tilde{p}(\varphi\Psi)_{yy} dydt+\int_0^{t_0}\int_{\mathbb{R}^-}\sigma\tilde{p}(\varphi\Psi)_{yy} dydt-\int_0^{t_0}\int_{\Omega_b}(D_\epsilon^{1-2q}\Psi_y)_y\tilde{p}\varphi dydt\\
&=\int_0^{t_0}\int_R^{R+1}\tilde{p}(\varphi_{yy}\Psi+2\varphi_y\Psi_y)dydt+\int_0^{t_0}\int_{-(R+1)}^{-R}\sigma\tilde{p}(\varphi_{yy}\Psi+2\varphi_y\Psi_y)dydt.
\end{aligned}$$

Thus, we have

$$\begin{aligned}
|p(t_0,y_0)| &\leq C\left(\int_0^{t_0}\int_R^{R+1}(|\Psi|+2|\Psi_y|)dydt+\int_0^{t_0}\int_{-(R+1)}^{-R}(|\Psi|+2|\Psi_y|)dydt\right)\\
&\to 0,
\end{aligned}$$

as $R\to 0$. Since $t_0>0$, $y_0\in\Omega_b$ is arbitrary, Problem (3.4) admits only the trivial solution. □

Next, we show the existence by solving (3.2) by gluing together two solutions of boundary value problems with appropriate interface conditions. First, we divide the real line into two regions, $\{y>0\}$ and $\{y<0\}$. Then, in the region $\{y>0\}$, (3.2) is written as

$$\begin{cases} p_t=p_{yy}, & t,y>0,\\ p(0,y)=p_0(y), & y>0,\\ p(t,0)=h(t), & t>0, \end{cases} \tag{3.6}$$

where $h(t)$ is treated as a given boundary value for now. In the region $\{y<0\}$, (3.2) is written as

$$\begin{cases} p_t=\sigma p_{yy} & t>0,\ y<0,\\ p(0,y)=p_0(y) & y<0,\\ p(t,0)=h(t) & t>0, \end{cases} \tag{3.7}$$

where $h(t)$ is the same boundary value. For any given boundary value, we may solve the problem and construct a solution p defined on $\mathbb{R}$. This will satisfy all conditions in Definition 2.1 except the continuity of the flux in (2.4). Therefore, it suffices to find an $h(t)$ that satisfies the continuity of the flux, i.e.,

$$\sigma p_y(t,0^-)=p_y(t,0^+). \tag{3.8}$$

In conclusion, the original problem (2.2) is written as a system (3.6)–(3.8).

The solution of (3.6) is explicitly given by

$$
\begin{aligned}
p(t,y) = &\int_0^\infty p_0(\xi)\Phi(t,y,\xi)\,d\xi \\
&+ \int_{0^+}^t h'(\tau)\mathrm{erfc}\Big(\frac{y}{2\sqrt{t-\tau}}\Big)\,d\tau + h(0^+)\mathrm{erfc}\Big(\frac{y}{2\sqrt{t}}\Big),
\end{aligned}
\qquad y>0, \tag{3.9}
$$

where

$$
\Phi(t,x,\xi) := \frac{1}{2\sqrt{\pi t}}\big(e^{-\frac{(x-\xi)^2}{4t}} - e^{-\frac{(x+\xi)^2}{4t}}\big)
$$

(see [7, Eq.(1.4.9) in p.19 and Eq.(1.4.21) in p.22] for example). To use the same formula for the solution of (3.7), we change the variables as

$$
s=\sigma t, \quad z=-y, \quad v(s,z)=p(t,y).
$$

Then, (3.7) turns into

$$
\begin{cases}
v_s = v_{zz} & s>0,\ z>0,\\
v(0,z) = p_0(-z) & z>0,\\
v(s,0) = h(\frac{s}{\sigma}) & s>0.
\end{cases}
$$

Therefore,

$$
\begin{aligned}
v(s,z) = &\int_0^\infty v(0,\xi)\Phi(s,z,\xi)\,d\xi \\
&+ \int_{0^+}^s \frac{h'(\frac{\tau}{\sigma})}{\sigma}\mathrm{erfc}\Big(\frac{z}{2\sqrt{s-\tau}}\Big)\,d\tau + h(0^+)\mathrm{erfc}\Big(\frac{z}{2\sqrt{s}}\Big).
\end{aligned}
$$

If we return to the original variables, we obtain

$$
\begin{aligned}
p(t,y) = &\int_0^\infty p_0(-\xi)\Phi(\sigma t,-y,\xi)\,d\xi \\
&+ \int_{0^+}^{\sigma t} \frac{h'(\frac{\tau}{\sigma})}{\sigma}\mathrm{erfc}\Big(\frac{-y}{2\sqrt{\sigma t-\tau}}\Big)\,d\tau + h(0^+)\mathrm{erfc}\Big(\frac{-y}{2\sqrt{\sigma t}}\Big),
\end{aligned}
\qquad y<0. \tag{3.10}
$$

The function $p(t,y)$ given by (3.9) and (3.10) satisfies (3.6) and (3.7), but not (3.8). The first step to find $h(t)$ that makes (3.8) to be satisfied is comparing the flux at the interface from the left and the right sides. For now, we assume that $h(t)$ satisfies regularities such that (3.9) and (3.10) are well-defined. The existence of a function $h(t)$ satisfying these assumptions will be carried out in Lemma 3.3.

Lemma 3.2. *Let $p(t,y)$ be given by* (3.9) *and* (3.10)*. Then,*

$$
\tfrac{\partial}{\partial y}p(t,0^+) = \int_0^\infty \tfrac{p_0(\xi)\xi}{2\sqrt{\pi t^3}}e^{-\frac{\xi^2}{4t}}\,d\xi - \int_{0^+}^t \tfrac{h'(\tau)}{\sqrt{\pi(t-\tau)}}\,d\tau - \tfrac{h(0^+)}{\sqrt{\pi t}}, \tag{3.11}
$$

$$
\tfrac{\partial}{\partial y}p(t,0^-) = -\int_0^\infty \tfrac{p_0(-\sqrt{\sigma}\xi)\xi}{2\sqrt{\pi\sigma t^3}}e^{-\frac{\xi^2}{4t}}\,d\xi + \int_{0^+}^t \tfrac{h'(\tau)}{\sqrt{\pi\sigma(t-\tau)}}\,d\tau + \tfrac{h(0^+)}{\sqrt{\pi\sigma t}}. \tag{3.12}
$$

Proof. First, calculate $\frac{\partial}{\partial y}p(t,y)$ for $y>0$ using (3.9),

$$\begin{aligned}\frac{\partial}{\partial y}p(t,y) = \; & \int_0^\infty \tfrac{p_0(\xi)}{4\sqrt{\pi t^3}}((\xi-y)e^{-\frac{(y-\xi)^2}{4t}} + (\xi+y)e^{-\frac{(y+\xi)^2}{4t}})\,d\xi \\ & -\int_{0^+}^t \tfrac{1}{\sqrt{\pi(t-\tau)}}h'(\tau)e^{-\frac{y^2}{4(t-\tau)}}\,d\tau - h(0^+)\tfrac{1}{\sqrt{\pi t}}e^{-\frac{y^2}{4t}}.\end{aligned} \tag{3.13}$$

Then, (3.11) is derived directly by taking the limit as $y\to 0^+$ in (3.13).

Next, calculate $\dfrac{\partial}{\partial y}p(t,y)$ for $y<0$ using (3.10),

$$\begin{aligned}\frac{\partial}{\partial y}p(t,y) = \; & \int_0^\infty \tfrac{p_0(-\xi)}{4\sqrt{\pi\sigma^3 t^3}}((\xi+y)e^{-\frac{(y+\xi)^2}{4\sigma t}} + (\xi-y)e^{-\frac{(y-\xi)^2}{4\sigma t}})\,d\xi \\ & -\int_{0^+}^{\sigma t} \tfrac{h'(\frac{\tau}{\sigma})}{\sigma}\tfrac{1}{\sqrt{\pi(\sigma t-\tau)}}e^{-\frac{y^2}{4(\sigma t-\tau)}}\,d\tau - h(0^+)\tfrac{1}{\sqrt{\pi\sigma t}}e^{-\frac{y^2}{4\sigma t}}.\end{aligned} \tag{3.14}$$

Taking the limit as $y\to 0^-$ in (3.14) gives

$$\frac{\partial}{\partial y}p(t,0^-) = \int_0^\infty \frac{p_0(-\xi)\xi}{2\sqrt{\pi\sigma^3 t^3}}e^{-\frac{\xi^2}{4\sigma t}}\,d\xi - \int_{0^+}^{\sigma t}\frac{h'(\frac{\tau}{\sigma})}{\sigma\sqrt{\pi(\sigma t-\tau)}}\,d\tau - \frac{h(0^+)}{\sqrt{\pi\sigma t}},$$

which implies (3.12) by taking change of variables $\xi' := \frac{\xi}{\sqrt{\sigma}}$ and $\tau' := \frac{\tau}{\sigma}$. $\square$

Next, we find the $h(t)$ that makes the flux continuous, i.e., (3.8) is satisfied. We also show the $h(t)$ is uniquely decided, and hence the solution of (2.2) is unique.

Lemma 3.3. *Let $\sigma>0$, $p_0\in C(\Omega_b)\cap L^\infty(\mathbb{R})$ with existing the limits $p(0^+)$ and $p(0^-)$, satisfying $p_0\geq 0$. Then, the function $p(t,y)$, defined by* (3.9) *and* (3.10)*, is well-defined and constitutes a solution of Problem* (3.2) *if and only if*

$$h(t) = \int_0^\infty \frac{p_0(\xi)+\sqrt{\sigma}p_0(-\sqrt{\sigma}\xi)}{1+\sqrt{\sigma}}\frac{e^{-\frac{\xi^2}{4t}}}{\sqrt{\pi t}}\,d\xi, \tag{3.15}$$

where h belongs to $C^1(\mathbb{R}^+)\cap C([0,\infty))\cap L^\infty(\mathbb{R}^+)$.

Proof. Suppose the function $p(t,y)$, given by (3.9) and (3.10), to be well-defined and a solution of (3.2). Then $h\in C(\mathbb{R}^+)\cap L^\infty(\mathbb{R}^+)$, and both $h(0^+)$ and h' exist. Putting the results (3.11), (3.12) into (3.8) gives

$$\int_{0^+}^t \frac{h'(\tau)}{\sqrt{\pi(t-\tau)}}\,d\tau + \frac{h(0^+)}{\sqrt{\pi t}} = \int_0^\infty \frac{p_0(\xi)+\sqrt{\sigma}p_0(-\sqrt{\sigma}\xi)}{(1+\sqrt{\sigma})}\frac{\xi}{2\sqrt{\pi t^3}}e^{-\frac{\xi^2}{4t}}\,d\xi. \tag{3.16}$$

Take the Laplace transform of (3.16) with respect to the variable t. Then, we obtain a formula

$$\mathcal{L}\{h\}(s) = \int_0^\infty \frac{p_0(\xi)+\sqrt{\sigma}p_0(-\sqrt{\sigma}\xi)}{1+\sqrt{\sigma}}\frac{e^{-\xi\sqrt{s}}}{\sqrt{s}}\,d\xi. \tag{3.17}$$

Finally, by taking the inverse of Laplace transform of (3.17), we have

$$h(t) = \int_0^\infty \frac{p_0(\xi) + \sqrt{\sigma} p_0(-\sqrt{\sigma}\xi)}{1+\sqrt{\sigma}} \frac{e^{-\frac{\xi^2}{4t}}}{\sqrt{\pi t}}\, d\xi.$$

To prove the lemma in the other direction, suppose that $h(t)$ is given by the formula (3.15). We deduce from the conditions for initial function p_0 that $h \in C(\mathbb{R}^+)$ and $h(0^+)$ exists, allowing us to conclude $h \in C([0,\infty))$. Furthermore, $h \in L^\infty(\mathbb{R}^+)$. Indeed, we have

$$|h(t)| \le \frac{\|p_0\|_{L^\infty(\mathbb{R}^+)} + \sqrt{\sigma}\|p_0\|_{L^\infty(\mathbb{R}^-)}}{1+\sqrt{\sigma}}, \quad \text{for all } t > 0.$$

Denote

$$g(t,\xi) := \frac{p_0(\xi) + \sqrt{\sigma} p_0(-\sqrt{\sigma}\xi)}{1+\sqrt{\sigma}} \frac{e^{-\frac{\xi^2}{4t}}}{\sqrt{\pi t}}.$$

Differentiating the integrand g with respect to $t > 0$, we have

$$\frac{\partial}{\partial t} g(t,\xi) = \frac{p_0(\xi) + \sqrt{\sigma} p_0(-\sqrt{\sigma}\xi)}{1+\sqrt{\sigma}} \Big(\frac{\xi^2}{4t^2} - \frac{1}{2t}\Big) \frac{e^{-\frac{\xi^2}{4t}}}{\sqrt{\pi t}}.$$

Since $\frac{p_0(\xi)+\sqrt{\sigma}p_0(-\sqrt{\sigma}\xi)}{1+\sqrt{\sigma}} \in L^\infty_\xi(\mathbb{R}^+)$ and $(\frac{\xi^2}{4t^2} - \frac{1}{2t})\frac{e^{-\frac{\xi^2}{4t}}}{\sqrt{\pi t}} \in C(\mathbb{R}^+; L^1_\xi(\mathbb{R}^+))$, we obtain that $\frac{\partial}{\partial t} g(t,\xi) \in C(\mathbb{R}^+; L^1_\xi(\mathbb{R}^+))$. Thus, we can interchange derivative and integral operators, such as

$$h'(t) = \frac{d}{dt}\int_0^\infty g(t,\xi)\, d\xi = \int_0^\infty \frac{\partial}{\partial t} g(t,\xi)\, d\xi,$$

which yields $h \in C^1(\mathbb{R}^+)$. Now, we can construct a solution p for Problem (3.2)–(3.8) using (3.9), (3.10), and (3.15). Then the function p satisfies all conditions in Definition 3.1, except for L^∞ boundedness. We note that $p_0 \in L^\infty(\mathbb{R})$ and $h \in L^\infty(\mathbb{R}^+)$. As $\|p\|_{L^\infty(\mathbb{R}^+\times\mathbb{R})} \le \|p_0\|_{L^\infty(\mathbb{R})} + \|h\|_{L^\infty(\mathbb{R}^+)}$, p also satisfies the L^∞ boundedness condition, establishing it as a solution of Problem (3.2). $\square$

We have established the existence and the uniqueness of a solution of Problem (3.2). In the next lemma, we show the additional regularity.

Lemma 3.4 (Extra regularity of the flux). *Let $p(t,y)$ be the solution defined in Lemma 3.3. Then, the flux $(D_\epsilon^{1-2q} p_y)$ is in $C^{0,1}(\mathbb{R}^+\times\mathbb{R})$, i.e.,*

$$\sigma \frac{\partial^2}{\partial y^2} p(t,0^-) = \frac{\partial^2}{\partial y^2} p(t,0^+) = h'(t).$$

Proof. Remember that $h(t) \in C^1(\mathbb{R}^+) \cap C([0,\infty))$ is already shown in the proof of Lemma 3.3. First, calculate $\frac{\partial^2}{\partial y^2}p(t,y)$ for $y > 0$:

$$\begin{aligned}&\tfrac{\partial^2}{\partial y^2}p(t,y)\\ &= \textstyle\int_0^\infty \frac{p_0(\xi)}{8\sqrt{\pi t^5}}\big(((\xi-y)^2-1)e^{-\frac{(y-\xi)^2}{4t}} - ((\xi+y)^2-1)e^{-\frac{(y+\xi)^2}{4t}}\big)\,d\xi \\ &\quad + \textstyle\int_{0^+}^t \frac{y}{2\sqrt{\pi(t-\tau)^3}}h'(\tau)e^{-\frac{y^2}{4(t-\tau)}}\,d\tau + h(0^+)\frac{y}{2\sqrt{\pi t^3}}e^{-\frac{y^2}{4t}}.\end{aligned}\tag{3.18}$$

Taking the limit of (3.18) as $y \to 0^+$ gives

$$\frac{\partial^2}{\partial y^2}p(t,0^+) = \lim_{y\to 0^+}\int_{0^+}^t \frac{y}{2\sqrt{\pi(t-\tau)^3}}h'(\tau)e^{-\frac{y^2}{4(t-\tau)}}\,d\tau.$$

After taking $\eta := \frac{y}{\sqrt{t-\tau}}$, the second-order derivative is written as

$$\frac{\partial^2}{\partial y^2}p(t,0^+) = \lim_{y\to 0^+}\int_{\frac{y}{\sqrt{t}}}^\infty \frac{1}{\sqrt{\pi}}h'\Big(t-\frac{y^2}{\eta^2}\Big)e^{-\frac{\eta^2}{4}}\,d\eta = h'(t).$$

Similarly, calculate $\frac{\partial^2}{\partial y^2}p(t,y)$ for $y < 0$:

$$\begin{aligned}&\tfrac{\partial^2}{\partial y^2}p(t,y)\\ &= \textstyle\int_0^\infty \frac{p_0(-\xi)}{8\sqrt{\pi\sigma^5 t^5}}\big(((\xi-y)^2-1)e^{-\frac{(y-\xi)^2}{4\sigma t}} - ((\xi+y)^2-1)e^{-\frac{(y+\xi)^2}{4\sigma t}}\big)\,d\xi \\ &\quad + \textstyle\int_{0^+}^t \frac{y}{2\sqrt{\pi\sigma^3(t-\tau)^3}}h'(\tau)e^{-\frac{y^2}{4\sigma(t-\tau)}}\,d\tau + h(0^+)\frac{y}{2\sqrt{\pi\sigma^3 t^3}}e^{-\frac{y^2}{4\sigma t}}.\end{aligned}\tag{3.19}$$

Taking the limit of (3.19) as $y \to 0^-$ gives

$$\frac{\partial^2}{\partial y^2}p(t,0^-) = \lim_{y\to 0^+}\int_{0^+}^t \frac{y}{2\sqrt{\pi\sigma^3(t-\tau)^3}}h'(\tau)e^{-\frac{y^2}{4\sigma(t-\tau)}}\,d\tau.$$

After taking $\eta := -\frac{y}{\sqrt{t-\tau}}$, the second-order derivative is written as

$$\frac{\partial^2}{\partial y^2}p(t,0^-) = \lim_{y\to 0^-}\int_{-\infty}^{\frac{y}{\sqrt{t}}} \frac{1}{\sqrt{\pi\sigma^3}}h'\Big(t-\frac{y^2}{\eta^2}\Big)e^{-\frac{\eta^2}{4\sigma}}\,d\eta = h'(t)/\sigma.$$

The comparison of the two second-order derivatives completes the proof. □

The lemmas 3.3 and 3.4 imply that the obtained solution $p(t,y)$ satisfies (3.2) in the classical sense. That means the differentiations in the equation (3.2) are valid even at the interface $x = 0$. The additional regularities expressed in (2.5) can be equivalently stated as the inclusions

$$p_t \in C(\mathbb{R}^+\times\mathbb{R}) \quad\text{and}\quad (D_\epsilon^{1-2q}p_y)_y \in C(\mathbb{R}^+\times\mathbb{R}),$$

which are implied by the inclusion $(D_\epsilon^{1-2q}p_y) \in C^{0,1}(\mathbb{R}^+\times\mathbb{R})$. These inclusions can be written as

$$p_t = D_\epsilon^q u_t \in C(\mathbb{R}^+\times\mathbb{R}),$$

and

$$(D_\epsilon^{1-2q}p_y)_y = D_\epsilon^q(D_\epsilon^{1-2q}D_\epsilon^q p_x)_x = D_\epsilon^q(D_\epsilon^{1-q}(D_\epsilon^q u)_x)_x \in C(\mathbb{R}^+\times\mathbb{R}).$$

Finally, we show the boundary behavior of the solution.

Lemma 3.5 (Boundary condition when $\epsilon \to 0$). *Let $\sigma \in \mathbb{R}^+$, $p_0 \in C(\Omega_b) \cap L^\infty(\mathbb{R})$, $p_0 \geq 0$, and $h(t;\epsilon)$ be given by (3.15). Then, $p(t,y;\epsilon)$ converges to a limit $U(t,y)$ for all $y > 0$ pointwise as $\epsilon \to 0$, and*

$$\begin{cases} \displaystyle\lim_{y\to 0+} \frac{\partial U}{\partial y}(t,y) = 0 & \text{if } q < 0.5, \\ \displaystyle\lim_{y\to 0+} \quad U(t,y) = 0 & \text{if } q > 0.5. \end{cases}$$

Furthermore, as $\epsilon \to 0$,

$$\begin{cases} \displaystyle\left|\frac{\partial p}{\partial y}(t,0^+;\epsilon)\right| = O(\epsilon^{0.5-q}) & \text{if } q < 0.5, \\ \quad |p(t,0^+;\epsilon)| = O(\epsilon^{q-0.5}) & \text{if } q > 0.5. \end{cases}$$

Proof. (i) Consider the case $q < 0.5$. Note that $\sigma = \epsilon^{1-2q} \to 0$ as $\epsilon \to 0$. First, we show the existence of a limit. By (3.15), for a fixed $t > 0$, we have

$$\lim_{\epsilon\to 0} h(t;\epsilon) = \int_0^\infty p_0(\xi) \frac{e^{-\frac{\xi^2}{4t}}}{\sqrt{\pi t}}\, d\xi,$$
$$\lim_{\epsilon\to 0} h'(t;\epsilon) = \int_0^\infty p_0(\xi) \Big(\frac{\xi^2}{4t^2} - \frac{1}{2t}\Big) \frac{e^{-\frac{\xi^2}{4t}}}{\sqrt{\pi t}}.$$

Hence $h(t;0^+) \in C^1(\mathbb{R}^+) \cap C([0,\infty))$. Therefore, taking the limit as $\epsilon \to 0$ in (3.9), we can see that $p(t,y;\epsilon)$ converges as $\epsilon \to 0$.

Next, we show the boundary behavior. By (3.11) and (3.16),

$$\begin{aligned} \frac{\partial p}{\partial y}(t,0^+;\epsilon) &= \int_0^\infty \frac{p_0(\xi)\xi}{2\sqrt{\pi t^3}} e^{-\frac{\xi^2}{4t}}\, d\xi - \int_{0^+}^t \frac{h'(\tau)}{\sqrt{\pi(t-\tau)}}\, d\tau - \frac{h(0^+)}{\sqrt{\pi t}} \\ &= \int_0^\infty \Big(p_0(\xi) - \frac{p_0(\xi) + \sqrt{\sigma} p_0(-\sqrt{\sigma}\xi)}{1+\sqrt{\sigma}}\Big) \frac{\xi}{2\sqrt{\pi t^3}} e^{-\frac{\xi^2}{4t}}\, d\xi \\ &= \int_0^\infty \frac{\sqrt{\sigma}(p_0(\xi) - p_0(-\sqrt{\sigma}\xi))}{1+\sqrt{\sigma}} \frac{\xi}{2\sqrt{\pi t^3}} e^{-\frac{\xi^2}{4t}}\, d\xi. \end{aligned}$$

Hence for a fixed $t > 0$,

$$\left|\frac{\partial p}{\partial y}(t,0^+;\epsilon)\right| \leq C \frac{\sqrt{\sigma}}{1+\sqrt{\sigma}} = O(\sqrt{\sigma}) = O(\epsilon^{0.5-q}).$$

(ii) Consider the case $q > 0.5$. Note that

$$\sigma = \epsilon^{1-2q} \to \infty \quad \text{and} \quad \|p_0\|_{L^\infty(\mathbb{R}^-)} = \epsilon^q \|\phi\|_{L^\infty(\mathbb{R}^-)} \to 0$$

as $\epsilon \to 0$. By (3.15), we have

$$
\begin{aligned}
|h(t;\epsilon)| &= \left| \int_0^\infty \frac{p_0(\xi) + \sqrt{\sigma} p_0(-\sqrt{\sigma}\xi)}{1+\sqrt{\sigma}} \frac{e^{-\frac{\xi^2}{4t}}}{\sqrt{\pi t}}\, d\xi \right| \\
&\le \frac{\|p_0\|_{L^\infty(\mathbb{R}^+)} + \sqrt{\sigma}\|p_0\|_{L^\infty(\mathbb{R}^-)}}{1+\sqrt{\sigma}} \\
&= \frac{\|p_0\|_{L^\infty(\mathbb{R}^+)}\epsilon^{q-0.5} + \epsilon^q \|\phi\|_{L^\infty(\mathbb{R}^-)}}{\epsilon^{q-0.5}+1} \\
&= O(\epsilon^{q-0.5}),
\end{aligned}
$$

as $\epsilon \to 0$. Similarly, we can check that $h'(t;\epsilon) \to 0$ uniformly as $\epsilon \to 0$. Therefore by (3.9),

$$
\lim_{\epsilon\to 0} p(t,y;\epsilon) = \int_0^\infty p_0(\xi)\Phi(t,y,\xi)\, d\xi
$$

for all $y > 0$. Hence, the limit exists. The boundary behavior is already proved because $|p(t,0^+;\epsilon)| = |h(t;\epsilon)| = O(\epsilon^{q-0.5})$. □

4. Explicit solutions

For special initial values, the value $h(t)$ at the interface is given in a simple form, and hence the solution $p(t,y)$ and the limit as $\epsilon \to 0$ are given in simpler forms. In this section, we present two cases of explicit solutions. These functions provide useful information and intuition about heterogeneous diffusion equation (2.2).

4.1. **Fundamental solution.**

We consider the explicit solution when the initial value is the delta distribution placed at $x_0 > 0$, i.e.,

$$
\phi(x) = \delta(x - x_0).
$$

Although $\phi \notin L^\infty$, we can construct the fundamental solution. First, we calculate the boundary value $h(t)$ using (3.15). We write the initial condition in terms of the potential variable p, which is

$$
p_0(y) = \delta(y - x_0).
$$

Putting this into (3.15) gives

$$
h(t) = \frac{e^{-\frac{x_0^2}{4t}}}{(1+\sqrt{\sigma})\sqrt{\pi t}}.
$$

Then, (3.9) and (3.10) gives the explicit solution

$$
p(t,y) = \begin{cases}
\Phi(t,y,x_0) + \frac{y}{2\sqrt{\pi}} \int_0^t \frac{1}{1+\sqrt{\sigma}} \frac{e^{-\frac{x_0^2}{4(t-\tau)}}}{\sqrt{\pi(t-\tau)}} \frac{e^{-\frac{y^2}{4\tau}}}{\sqrt{\tau^3}}\, d\tau, & y > 0, \\
-\frac{y}{2\sqrt{\pi}} \int_0^t \frac{1}{\sqrt{\sigma}(1+\sqrt{\sigma})} \frac{e^{-\frac{x_0^2}{4(t-\tau)}}}{\sqrt{\pi(t-\tau)}} \frac{e^{-\frac{y^2}{4\sigma\tau}}}{\sqrt{\tau^3}}\, d\tau, & y < 0.
\end{cases}
$$

After a simplification, we obtain the fundamental solution of (2.2),

$$p(t,y)=\begin{cases}\frac{1}{2\sqrt{\pi t}}e^{-\frac{(y-x_0)^2}{4t}}+\frac{1-\sqrt{\sigma}}{2(1+\sqrt{\sigma})}\frac{1}{\sqrt{\pi t}}e^{-\frac{(y+x_0)^2}{4t}}, & y>0,\\ \frac{1}{(1+\sqrt{\sigma})\sqrt{\pi t}}e^{-\frac{(x_0-\frac{y}{\sqrt{\sigma}})^2}{4t}}, & y<0.\end{cases} \tag{4.1}$$

The limit of the solution as $\epsilon\to 0$ is divided into three cases. If $q>0.5$, $\sigma\to\infty$ as $\epsilon\to 0$. Then, $p(t,y)$ in (4.1) converges to

$$p(t,y)=\begin{cases}\frac{1}{2\sqrt{\pi t}}e^{-\frac{(y-x_0)^2}{4t}}-\frac{1}{2\sqrt{\pi t}}e^{-\frac{(y+x_0)^2}{4t}}, & y>0,\\ 0, & y<0.\end{cases}$$

One can easily check that $p(t,0^+)=0$ and $p_y(t,0^+)\neq 0$ in the case. If $q<0.5$, then $\sigma\to 0$ as $\epsilon\to 0$, and $p(t,y)$ in (4.1) converges to

$$p(t,y)=\begin{cases}\frac{1}{2\sqrt{\pi t}}e^{-\frac{(y-x_0)^2}{4t}}+\frac{1}{2\sqrt{\pi t}}e^{-\frac{(y+x_0)^2}{4t}}, & y>0,\\ 0, & y<0.\end{cases}$$

One can easily check that $p(t,0^+)\neq 0$ and $p_y(t,0^+)=0$ in the case.

The third case of $q=0.5$ is special. In this case, $\sigma=1$ for all $\epsilon>0$. Hence, the solution in (4.1) is independent of ϵ. In fact, the variable y fully absorbed the effect of the heterogeneity. Then, $p(t,y)$ in (4.1) is written as

$$p(t,y)=\frac{1}{2\sqrt{\pi t}}e^{-\frac{(y-x_0)^2}{4t}},\quad y\in\mathbb{R},$$

which is the heat kernel on the whole real line $\mathbb{R}$. One can easily check that $p(t,0^+)\neq 0$ and $p_y(t,0^+)\neq 0$ in the case. Both Neumann and Dirichlet boundary conditions fail when $q=0.5$.

4.2. **Step function initial value.** We consider the explicit solution when the initial value is a step function,

$$\phi(x)=\begin{cases}a, & x>0,\\ b, & x<0.\end{cases}$$

Then, the corresponding initial value for the potential p is

$$p_0(x)=\begin{cases}a, & x>0,\\ \epsilon^q b, & x<0.\end{cases}$$

Putting this initial value into (3.15) gives

$$h(t)=\frac{a+\epsilon^q b}{1+\sqrt{\sigma}}.$$

Then, (3.9) gives the explicit solution

$$p(t,y)=\begin{cases}a\left(1-\mathrm{erfc}\left(\frac{y}{2\sqrt{t}}\right)\right)+\frac{a+\epsilon^q b}{1+\sqrt{\sigma}}\mathrm{erfc}\left(\frac{y}{2\sqrt{t}}\right), & y>0,\\ \epsilon^q b\left(1-\mathrm{erfc}\left(\frac{-y}{2\sqrt{\sigma t}}\right)\right)+\frac{a+\epsilon^q b}{1+\sqrt{\sigma}}\mathrm{erfc}\left(\frac{-y}{2\sqrt{\sigma t}}\right), & y<0.\end{cases}$$

After a simplification, we obtain the solution of (2.2),

$$p(t,y)=\begin{cases} a+\frac{\epsilon^q b-\sqrt{\sigma}a}{1+\sqrt{\sigma}}\frac{2}{\sqrt{\pi}}\int_{\frac{y}{2\sqrt{t}}}^{\infty}e^{-\eta^2}\,d\eta, & y>0,\\ \epsilon^q b+\frac{a-\sqrt{\sigma}\epsilon^q b}{1+\sqrt{\sigma}}\frac{2}{\sqrt{\pi}}\int_{\frac{-y}{2\sqrt{\sigma t}}}^{\infty}e^{-\eta^2}\,d\eta, & y<0.\end{cases} \tag{4.2}$$

The limit of the solution as $\epsilon\to 0$ is divided into three cases. If $q>0.5$, $\sigma\to\infty$ as $\epsilon\to 0$. Then, $p(t,y)$ in (4.2) converges to

$$p(t,y)=\begin{cases} a-a\frac{2}{\sqrt{\pi}}\int_{\frac{y}{2\sqrt{t}}}^{\infty}e^{-\eta^2}\,d\eta, & y>0,\\ 0 & y<0.\end{cases}$$

If $q<0.5$, $\sigma\to 0$ as $\epsilon\to 0$, and $p(t,y)$ in (4.2) converges to

$$p(t,y)=\begin{cases} a, & y>0,\\ 0, & y<0.\end{cases}$$

If $q=0.5$, $\sigma=1$ for all $\epsilon>0$, and $p(t,y)$ in (4.2) converges to

$$p(t,y)=\begin{cases} a-\frac{a}{\sqrt{\pi}}\int_{\frac{y}{2\sqrt{t}}}^{\infty}e^{-\eta^2}\,d\eta, & y>0,\\ \frac{a}{\sqrt{\pi}}\int_{\frac{-y}{2\sqrt{t}}}^{\infty}e^{-\eta^2}\,d\eta, & y<0.\end{cases}$$

5. Numerical test

In this section, we test the boundary condition (2.6) and the decay rate (2.7) numerically. Solving (2.2) directly is tricky due to the discontinuity of the solution u at the interface $x=0$. One way to handle the discontinuity is to write it in terms of pressure,

$$p(t,x):=D_\epsilon^q u(t,x).$$

Then, (2.2) is written as

$$\begin{cases} D_\epsilon^{-q}p_t=(D_\epsilon^{1-q}p_x)_x, & t>0,\ x\in\mathbb{R},\\ p(0,x)=D_\epsilon^q\phi(x), & x\in\mathbb{R}.\end{cases} \tag{5.1}$$

We may solve (5.1) for $p(t,x)$ and then return to $u(t,x)$. Note that both equations, (3.2) and (5.1), are for the same diffusion pressure $p=D_\epsilon^q u$, where the difference is in the space variables x and y.

Four snapshots of solutions of the two cases, $u(t,x)$ and $p(t,y)$, are given in Figure 1, when

$$\phi(x)=1,\quad \Delta x=0.002,\quad \text{and}\quad q=0.9.$$

We used a Matlab function, 'pdepe', for the computation. The snapshots are taken at the moment $t=0.01$ for four cases with $\epsilon=2^{-k}$ with $k=1,2,3,$ and 4. According to the variable changes, $u=p$ in the region $x>0$, which can be observed in the figures.

We observe that the boundary values $u(t,0^+)\to 0$ as $\epsilon\to 0$. However, we could not decrease ϵ further when we solve (5.1) numerically. It requires a smaller mesh size. On the other hand, solving (3.2) is handier as long as

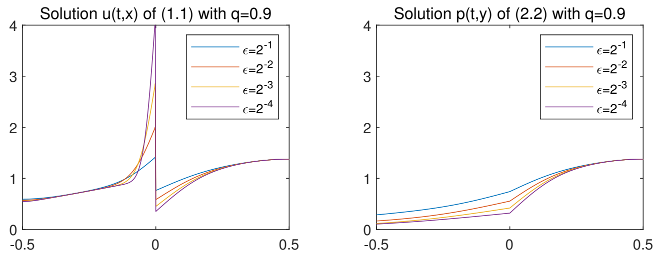


FIGURE 1. Snapshots at $t = 0.01$ are identical for $x, y > 0$.

the domain for $y < 0$ is taken properly. The boundary values $u(t, 0^+)$ are displayed as $\epsilon \to 0$ in the left of Figure 2. The boundary value $u(t, 0^+)$ is computed for 50 cases of $\epsilon \in (10^{-4}, 10^0)$ in a log scale. We can observe that they make a line of slope $k = 0.39$ for the case $q = 0.9$. This implies that the relation between the boundary value and the parameter ϵ is approximately

$$u(t, 0^+) = O(\epsilon^k) \quad \text{with} \quad k \cong 0.39 \quad \text{if} \quad q = 0.9.$$

On the other hand, the graph for the case $q = 0.6$ is slightly curved. If we take the parameter regime $10^{-4} < \epsilon < 10^{-2}$, we have

$$u(t, 0^+) = O(\epsilon^k) \quad \text{with} \quad k \cong 0.082 \quad \text{if} \quad q = 0.6.$$

This shows that the boundary value goes to zero slowly when q is close to 0.5. In the third figure, the power k is computed for 50 cases of $q \in (0.5, 1)$. We can see that $k \to 0$ as $q \to 0.5$ almost linearly. The numerical observations agree with our decay estimate (2.7), which is $k \simeq q - 0.5$.

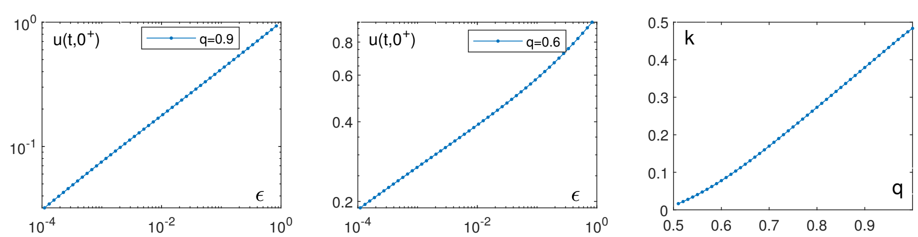


FIGURE 2. Power laws between $u(t, 0^+)$ and ϵ when $\epsilon \to 0$.

Four snapshots of solutions of (3.2) are given in Figure 3 when

$$\phi(x) = 1 + \sin(x), \quad \Delta x = 0.002, \quad \text{and} \quad q = 0.1.$$

The snapshots are taken at the moment $t = 0.1$ for four cases with $\epsilon = 10^{-k}$ with $k = 0, 1, 2$, and 3. The left figure is for the solution density $u(t, x)$. The boundary value increases as $\epsilon \to 0$. The second figure is for the gradient of the solution $\partial_x u(t, x)$. We can observe that the derivative $\partial_x u(t, 0^+)$ decreases to 0 as $\epsilon \to 0$.

In the left of Figure 4, the slopes of the solution at the boundary, $\partial_x u(t, 0^+)$, are given as $\epsilon \to 0$. The graph consists of 50 cases of $\epsilon \in (10^{-4}, 10^0)$ in a

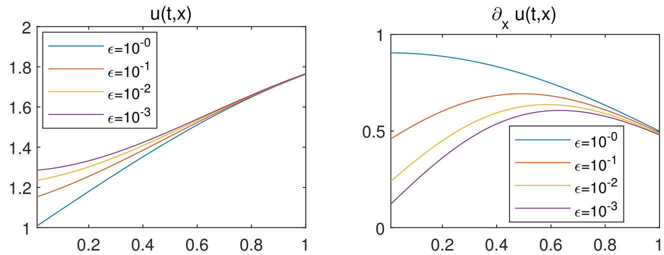


FIGURE 3. Snapshots at $t = 0.1$. Slope approaches 0 as $\epsilon \to 0$.

log scale. We can observe that they make almost a line of slope $k = 0.34$ for the case $q = 0.1$. This implies that the relation between the boundary slope and the parameter ϵ is

$$\partial_x u(t, 0^+) = O(\epsilon^k) \quad \text{with} \quad k \cong 0.34 \quad \text{if} \quad q = 0.1.$$

On the other hand, the graph for the case $q = 0.4$ is curved. If we take the parameter regime $10^{-4} < \epsilon < 10^{-3}$, we have

$$\partial_x u(t, 0^+) = O(\epsilon^k) \quad \text{with} \quad k \cong 0.063 \quad \text{if} \quad q = 0.4.$$

These numerical simulations show that the boundary slope goes to zero slower when q approaches 0.5. In the third figure, the power k is computed for 50 cases of $q \in (0, 0.5)$. We can see that $k \to 0$ as $q \to 0.5$ almost linearly. The numerical observations agree with our decay estimate (2.7), which suggests $k \simeq 0.5 - q$.

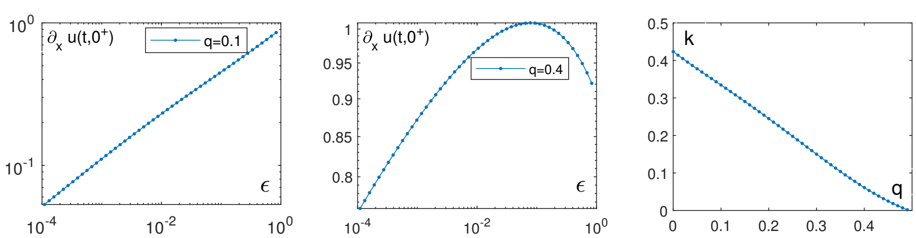


FIGURE 4. Power laws between $\partial_x u(t, 0^+)$ and ϵ when $\epsilon \to 0$.

6. WHY IS THE BOUNDARY CONDITION SPLIT AT $q = 0.5$?

Theorem 2.1 says that the Neumann boundary condition emerges as $\epsilon \to 0$ when $q < 0.5$, and the Dirichlet boundary condition when $q > 0.5$. The reason why the boundary condition splits along the case $q = 0.5$ can be explained using a random walk model. In a one-dimensional position jump process, particles jump walk length $\triangle x$ every sojourn time $\triangle t$ toward a randomly chosen direction. If $\triangle x$ and $\triangle t$ are constant, the diffusivity is constant and given by

$$D = \frac{(\triangle x)^2}{2\triangle t}.$$

If $\triangle x$ and $\triangle t$ converge to zero keeping the ratio D unchanged, the particle density $u(t,x)$ satisfies a diffusion equation

$$u_t = Du_{xx}. \tag{6.1}$$

Equation (6.1) is equivalent to (2.2) for any $q \in \mathbb{R}$ when D is constant.

To obtain the nonconstant diffusivity D in (1.3), we consider a reversible random walk system taking nonconstant $\triangle x$ and $\triangle t$. Diffusion equations for such spatially heterogeneous cases have been recently studied in [2, 8, 9]. Let $\delta > 0$ be a small constant, ℓ and τ be positive functions defined on $\mathbb{R}$, and

$$\triangle x\big|_{\text{at } x} = \ell(x)\delta \quad \text{and} \quad \triangle t\big|_{\text{at } x} = \tau(x)\delta^2.$$

Then, the corresponding heterogeneous diffusivity is

$$D(x) = \frac{\ell^2(x)}{2\tau(x)},$$

and the diffusion equation obtained after taking $\delta \to 0$ limit is

$$u_t = \frac{1}{2}\big(K\big(Mu\big)_x\big)_x, \quad K = \ell,\ M = \frac{\ell}{\tau}. \tag{6.2}$$

If τ is constant, the diffusion equation (6.2) is equivalent to (2.2) with $q = 0.5$. This is why the case $q = 0.5$, Wereide's diffusion law, is the border case. The corresponding exponent $q \in \mathbb{R}$ depends on the heterogeneity in $\triangle t$, and there is no universal one but different in each case.

There is an essential difference between the sojourn time $\triangle t$ and the walk length $\triangle x$. For example, a change of $\triangle x$ in the region $x < 0$ does not make any difference in the other region $x > 0$. For example, we have changed the scale of the space variable using the relation (3.1), which corresponds to the change of $\triangle x$ in the region $x < 0$. However, it does not change the density in the region $x > 0$, as we can see in Figure 1. On the other hand, if $\triangle t$ changes in the $x < 0$ region, the particle density in the $x > 0$ region changes.

Next, we consider the relation between τ and q. Let

$$\ell(x) = \begin{cases} \eta, & x \le 0, \\ 1, & x \ge 0, \end{cases} \qquad \tau(x) = \begin{cases} \zeta, & x \le 0, \\ 0.5, & x \ge 0. \end{cases}$$

Then, the diffusivity is given by

$$D(x) = \begin{cases} \frac{\eta^2}{2\zeta}, & x < 0, \\ 1, & x > 0. \end{cases}$$

To obtain the diffusivity in (1.3), we choose ζ and η so that $\frac{\eta^2}{2\zeta} = \epsilon$. If we take $\zeta = 0.5$, the diffusion law (6.2) corresponds to the case $q = 0.5$. For general $q \in \mathbb{R}$, relations among ϵ, ζ, η, and q are

$$\epsilon^{1-q} = \eta \quad \text{and} \quad \epsilon^q = \frac{\eta}{\zeta}.$$

Therefore, $\zeta = \epsilon^{1-2q}$. In other words, the parameter σ is actually the sojourn time ζ in the $x < 0$ region. If $q < 0.5$, $\zeta \to 0$ as $\epsilon \to 0$. This implies that the particles in $x < 0$ region jump so frequently as $\epsilon \to 0$ and hence collide the interface $x = 0$ infinitely times more frequently from the region $x < 0$. This makes particles in $x > 0$ cannot leave the region after taking the limit as $\epsilon \to 0$, which gives the Neumann boundary condition. On the other hand, if $q > 0.5$, $\zeta \to \infty$ as $\epsilon \to 0$. In this case, particles do not hit the interface $x = 0$ from the left side almost surely. Therefore, there is no chance for a particle that left the $x > 0$ region to return to it. This gives the zero-Dirichlet boundary condition. Note that the diffusion law (6.2) is behind the match between ζ and σ, and the exact bisection of the divided boundary condition regimes across $q = 0.5$.

Acknowledgements. J.C. was supported by the KERI Primary research program of MSIT/NST (No. 23A01002). Y.J.K. was supported by the National Research Foundation of Korea (NRF-2017R1A2B2010398).

References

[1] Sydney Chapman, *On the Brownian displacements and thermal diffusion of grains suspended in a non-uniform fluid*, Proc. Roy. Soc. Lond. A **119** (1928), 34–54.

[2] J. Chung, Y.-J. Kim, and M. Lee, Random walk with heterogeneous sojourn times, preprint (http://amath.kaist.ac.kr/papers/Kim/33.pdf).

[3] A. Fick, *On liquid diffusion*, Phil. Mag. **10** (1855), 30–39.

[4] D. Hilhorst, S.-M. Kang, H.-Y. Kim, and Y.-J. Kim, Fick's law selects the Neumann boundary condition, arXiv:2308.00321 (2023),

[5] N.G. Van Kampen, Itô versus Stratonovich. Journal of Statistical Physics, 24 (1981), 175–187.

[6] N.G. Van Kampen, Diffusion in inhomogeneous media. J. Phys. Chem. Solids 49, 673–677 (1988).

[7] J. Kevorkian, Partial Differential Equations: Analytical Solution Techniques (2nd ed.), Springer-Verlag, New York, 2000.

[8] H.-Y. Kim, Y.-J. Kim, and H.-J. Lim, Heterogeneous discrete kinetic model and its diffusion limit, Kinetic and Related Models 14(5) (2021), 749–765.

[9] Y.-J. Kim and H.-J. Lim, Heterogeneous discrete-time random walk and reference point dependency, preprint (2023).

[10] P.T. Landsberg, D grad v or grad(Dv)?, J. Appl. Phys. 56(1998), 1119.

[11] B.P. Van Milligen, P.D. Bons, B.A. Carreras, and R. Śnchez, R. On the applicability of Fick's law to diffusion in inhomogeneous systems. Eur. J. Phys. 26, 913–925 (2005).

[12] R. Sattin, Fick's law and Fokker–Planck equation in inhomogeneous environments. Phys. Lett. A 372, 3941–3945 (2008).

[13] Schnitzer, M. J. Theory of continuum random walks and application to chemotaxis. Phys. Rev. E 48, 2553 (1993).

[14] M. Wereide, *La diffusion d'une solution dont la concentration et la temperature sont variables*, Ann. Physique **2** (1914), 67–83.

[15] Friedman, A, Partial Differential Equations of Parabolic Type ([edition missing]). Dover Publications (2013).

(Jaywan Chung) Energy Conversion Research Center, Korea Electrotechnology Research Institute, 12, Jeongiui-gil, Changwon-si, Gyeongsangnam-do, 51543, Korea

Email address: jchung@keri.re.kr

(Seungmin Kang) Department of Mathematical Sciences, KAIST,e 291 Daehak-ro, Yuseong-gu, Daejeon, 34141, Korea

Email address: sngmn20@gmail.com

(Ho-Youn Kim) Computer, Electrical and Mathematical Science and Engineering Division, King AbdullahUniversity of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

Email address: ghsl0615@gmail.com

(Yong-Jung Kim) Department of Mathematical Sciences, KAIST,e 291 Daehak-ro, Yuseong-gu, Daejeon, 34141, Korea

Email address: yongkim@kaist.edu