MODELLING WITH MEASURES: APPROXIMATION OF A MASS-EMITTING OBJECT BY A POINT SOURCE

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ABSTRACT. We consider a linear diffusion equation on $\Omega := \mathbb{R}^2 \setminus \overline{\Omega_{\mathcal{O}}}$, where $\Omega_{\mathcal{O}}$ is a bounded domain. The time-dependent flux on the boundary $\Gamma := \partial\Omega_{\mathcal{O}}$ is prescribed. The aim of the paper is to approximate the dynamics by the solution of the diffusion equation on the whole of $\mathbb{R}^2$ with a measure-valued point source in the origin and provide estimates for the quality of approximation. For all time t, we derive an $L^2([0,t]; L^2(\Gamma))$-bound on the difference in flux on the boundary. Moreover, we derive for all $t > 0$ an $L^2(\Omega)$-bound and an $L^2([0,t]; H^1(\Omega))$-bound for the difference of the solutions to the two models.

1. **Introduction.** "What is the force on a test charge due to a single point charge q which is at rest a distance r away?" is a common type of question in textbooks about electromagnetism (e.g. [12], p. 59). In reality there is of course no such thing as a point charge having no volume. This is just a simplification due to the fact that the volume of the charged particle is very small compared to the other typical length scales in the system. Throughout physics it is common practice to replace objects of negligible size by point masses. For instance, grains or colloids in a solution [18], crowd dynamics [13], electrostatics [17], defects in crystalline structures [6, 24]. Of particular interest is the setting in which the exchange of mass, energy etc. between the interior and the exterior of the object takes place at its boundary. In this case the object is approximated not by a mere point mass, but by a point source. Experimental evidence suggests that this example of 'modelling with measures' is often a good approximation to the original (spatially extended)

system. In this paper, we consider the problem of quantifying the accuracy of this type of approximation, focussing on a simple scenario.

In $\mathbb{R}^2$, we consider an object of fixed shape and position and of finite size. Outside the object there is a concentration of mass that evolves by diffusion. On the boundary of the object there is prescribed mass flux in normal direction. This flux is a simplistic way of describing the result of processes that occur in the interior of the object. We wish to approximate this object by a point source. To this aim we replace the original diffusion equation on the exterior domain Ω by a diffusion equation on the whole of $\mathbb{R}^2$ with a Dirac measure included at its right-hand side. The exact formulation of the equations will be made clear in Section 2.

This is a first step towards modelling and analysing the mass distribution dynamics in realistic settings involving a large number of small objects moving around in a bounded domain while exchanging mass. Our motivation comes from the intracellular transport of chemical compounds in vesicles, like neurotransmitters in neurons (cf. [22]) or the hypothetical vesicular transport mechanism for the plant hormone auxin proposed in [2] as an alternative to the conventional auxin transport paradigm (in analogy to neurotransmitters). Auxin is a crucial molecule regulating growth and shape in plants. The vesicles are small membrane-bound balls covered by specific transmembrane transporter proteins that take up auxin from the surrounding cytoplasm. The vesicles are driven by molecular motors over a network of intracellular filaments [16, 27], e.g. from one end of the cell to the other as in Polar Auxin Transport (PAT). Experimental investigations of PAT in *Chara* species [5] revealed that neither diffusion nor cytoplasmic streaming can be the driving mechanism of PAT in the long (3-8 cm) internodal *Chara* cells. See [5, 27] for further discussion and an overview.

A substantial amount of mathematical modelling efforts on PAT have focussed on pattern formation in plant cell tissues (see [3, 19, 23] and the references cited therein). Upscaling to an effective macroscopic continuum description for transport at tissue level was considered in [7]. All models are based however on the assumption of diffusion as intracellular transport mechanism for auxin. Ultimately, we aim at obtaining a convenient mathematical description of the vesicle-driven transport dynamics *within* a cell, in particular in terms of an effective continuum model, which is needed to replace diffusion in an upscaling argument similar to [7]. In view of (the absence of) relevant mathematical literature, this perspective seems to be rather unexplored.

Why do we insist on introducing measures to this problem? This modelling strategy is especially useful once we wish to describe the interaction between multiple moving objects (vesicles). We expect the mathematical description to be much simpler in terms of discrete measures (i.e. the weighted sum of Dirac measures) and the analysis and numerical approximation likewise (see, for instance, [29, 30] for a related case). But before we can go to this advanced setting, we first need to investigate the quality of the approximation for a simple reference scenario; this is the main concern of this paper.

After the aforementioned overview of model equations in Section 2, we summarize in Section 3 the main (boundedness) results of this paper, followed by some useful preliminaries in Section 4. In Section 6 we show boundedness of the difference in the flux of the full problem (including the finite-size object) and the flux of the reduced problem (including the point source). This result is used in Section 7, where we estimate the difference between the two problems' solutions on the exterior domain.

2. **Two problems.** Let $\Omega_{\mathcal{O}} \in \mathbb{R}^2$ be an open and bounded domain, such that its boundary $\Gamma := \partial\Omega_{\mathcal{O}}$ is C^2 and has finite length. This set denotes the interior of an object $\mathcal{O}$ with mass-exchange at its boundary. We assume $0 \in \Omega_{\mathcal{O}}$. Let Ω denote the exterior of $\mathcal{O}$. That is, $\Omega := \mathbb{R}^2 \setminus \overline{\Omega_{\mathcal{O}}}$. See Figure 1a for a sketch of the geometry.

For given initial condition $u_0 : \Omega \to \mathbb{R}^+$ and given flux $\phi : \Gamma \times [0,T] \to \mathbb{R}$, we consider the problem

$$\begin{cases} \dfrac{\partial u}{\partial t} = d\Delta u, & \text{on } \Omega \times \mathbb{R}^+; \\ u(0) = u_0, & \text{on } \Omega; \\ d\nabla u \cdot n = \phi, & \text{on } \Gamma \times \mathbb{R}^+. \end{cases} \tag{1}$$

Here, $d > 0$ denotes the diffusion coefficient, which is fixed throughout this paper. The vector n denotes the unit normal pointing outwards on Γ (so *into* $\Omega_{\mathcal{O}}$), and ϕ is the *influx* of u w.r.t. Ω. Positive ϕ corresponds to flux in the direction of $-n$.

Use $v_0 : \overline{\Omega_{\mathcal{O}}} \to \mathbb{R}^+$ to define $\hat{u}_0 : \mathbb{R}^2 \to \mathbb{R}^+$, given by

$$\hat{u}_0 := \begin{cases} u_0, & \text{on } \Omega; \\ v_0, & \text{on } \overline{\Omega_{\mathcal{O}}}, \end{cases} \tag{2}$$

which is an extension of u_0 to the whole of $\mathbb{R}^2$. The aim of the paper is to quantify the quality of approximation of the solution of (1) (with an appropriate solution concept, see Section 5 below) with the restriction to Ω of the *mild solution* of the problem

$$\begin{cases} \dfrac{\partial \hat{u}}{\partial t} = d\Delta \hat{u} + \bar{\phi}\delta_0, & \text{on } \mathbb{R}^2 \times \mathbb{R}^+; \\ \hat{u}(0) = \hat{u}_0, & \text{on } \mathbb{R}^2, \end{cases} \tag{3}$$

(see also Section 5).

Remark 1. Typically, $\mathcal{O}$ is *small* (we are deliberately vague in what sense), but even if that is not the case, the approach of this paper gives information about how much the solutions of the two problems deviate on Ω. It is not our objective to investigate the behaviour of (1) in the limit $|\mathcal{O}| \to 0$. $\mathcal{O}$ keeps physical proportions.

Remark 2. In (3), we have introduced a mapping $\bar{\phi} : \mathbb{R}^+ \to \mathbb{R}$ which represents the magnitude of the mass source. A measure-valued source was treated, for instance, in [30] (in the context of numerical approximation schemes) or in [4]; see also [21] for more background on the solvability of such evolution equations.

Remark 3. Problem (3) is posed on the whole of $\mathbb{R}^2$. The boundary Γ has no physical meaning in this problem; see Figure 1b. However, the flux on this imaginary curve will be used in later estimates.

3. **Summary of the main results.** In Section 5 we shall use available results on maximal regularity that establish the existence of a unique solution u to Problem (1) in the sense of $L^2(\Omega)$-valued distributions, provided the initial condition $u_0 \in H^1(\Omega)$ and the prescribed flux $\phi \in H^1([0,T], L^2(\Gamma)) \cap L^2([0,T], H^1(\Gamma))$. Mild solutions to Problem (3) exist in a suitable Banach space containing the finite Borel measures for any initial *measure*, provided $\bar{\phi} \in L^1_{\text{loc}}(\mathbb{R}^+)$ (see Section 5). We show that for more regular initial condition $\hat{u}_0 \in H^1(\mathbb{R}^2)$ and flux from the source $\bar{\phi} \in H^1([0,T])$, the restriction of the mild solution $\hat{u}$ to Ω is as regular as u on Ω (Theorem 5.2), namely

$$u, \hat{u} \in H^1([0,T], L^2(\Omega)) \cap L^2([0,T], H^2(\Omega)).$$

(A) Original domain   (B) Extended domain
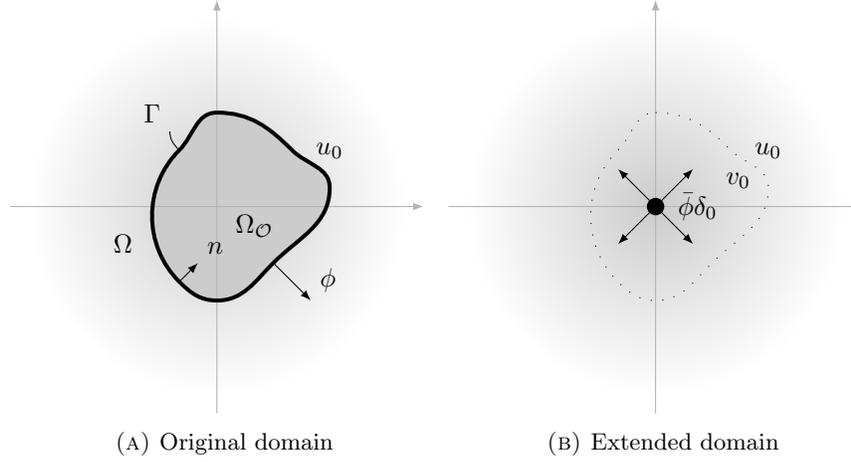
FIGURE 1. (A): Typical example of the original domain Ω outside the object $\mathcal{O}$, on which u evolves according to (1) starting from initial condition u_0. Also, ϕ and n, related to the boundary condition on Γ, are indicated. (B): Domain for the reduced problem associated to (A). Γ is now an imaginary curve within the domain (to be used later). The initial conditions u_0 and v_0 hold outside and inside Γ, respectively. The point source of magnitude $\bar{\phi}$ is indicated in the origin.

Consequently, the time-integrated deviation between the prescribed flux ϕ on Γ in Problem (1) and the flux on Γ generated by the solution to Problem (3) with flux $\bar{\phi}$ at 0, i.e.

$$c^*(t) := \int_0^t \|\phi(\tau) - d\nabla\hat{u}(\tau) \cdot n\|_{L^2(\Gamma)}^2 \, d\tau \tag{4}$$

is finite for all $t \geq 0$. In Section 6 we derive an upper bound on $c^*(t)$, see Theorem 6.3 in terms of the data for Problems (1) and (3).

Our main result is the following:

Theorem 3.1. *Let $T > 0$ and let the data for Problems (1) and (3) satisfy $u_0 \in H^1(\Omega)$, $\phi \in H^1([0,T], L^2(\Gamma)) \cap L^2([0,T], H^1(\Gamma))$, $\bar{\phi} \in H^1([0,T])$ and $\hat{u}_0 \in H^1(\mathbb{R}^2)$ is such that $\nabla\hat{u}_0 \in L^p(\mathbb{R}^2)$ for some $2 < p < \infty$. Then the unique solutions u and $\hat{u}$ to (1) and (3) are such, that for all $\varepsilon \in (0, 2d)$ there are $c_1, c_2 > 0$ such that*

$$\|u(\cdot, t) - \hat{u}(\cdot, t)\|_{L^2(\Omega)}^2 \leq c_1 \, c^*(t) \, e^{\varepsilon t}, \text{ and} \tag{5}$$

$$\int_0^t \|u - \hat{u}\|_{H^1(\Omega)}^2 \leq c_2 \, c^*(t) \, e^{\varepsilon t}. \tag{6}$$

for all $0 < t \leq T$. The constants depend on Ω, d and ε.

Remark 4. Note that the initial condition $\hat{u}_0$ needs to be more regular than 'just' $H^1(\mathbb{R}^2)$ as needed in the regularity result for $\hat{u}$. The flux estimates in Section 6 require $\nabla\hat{u}_0 \in L^p(\mathbb{R}^2)$ with $2 < p < \infty$. The Sobolev Embedding Theorem (cf. [1], Thrm. 4.12, p. 85) yields that $\hat{u}_0 \in H^2(\mathbb{R}^2)$ is a sufficient condition to have the stronger result that $\hat{u}_0 \in H^1(\mathbb{R}^2) \cap W^{1,p}(\mathbb{R}^2)$ for any $2 < p < \infty$. In that case necessarily $u_0 \in H^2(\Omega)$ too.

An important characteristic of estimates (5) and (6) is that the upper bounds are linear in $c^*(t)$. This implies that, if we manage to enforce $c^*(t)$ to be small, then also the solutions u and $\hat{u}$ are close (in the sense described above) on Ω. At this point, we manage only to get a rough bound on $c^*(t)$, cf. Theorem 6.3, but we conjecture that a more sophisticated estimate is possible; see Section 8.

4. **Preliminaries.** We need a few fundamental results, before we can discuss the properties of solutions (Section 5) and the details of our results (Section 6 and further). We summarize these preliminaries in this section.

Lemma 4.1 (Properties of the convolution, [11] Propositions 8.8 and 8.9, p. 241)**.** *Let $p, q \geq 1$ be such that $1/p + 1/q = 1$. If $f \in L^p(\mathbb{R}^n)$ and $g \in L^q(\mathbb{R}^n)$, then*

1. *$(f * g)(x)$ exists for all $x \in \mathbb{R}^n$;*
2. *$f * g$ is bounded and uniformly continuous;*
3. *$\|f * g\|_{L^\infty(\mathbb{R}^n)} \leq \|f\|_{L^p(\mathbb{R}^n)} \|g\|_{L^q(\mathbb{R}^n)}$.*

If moreover $p, q \in (1, \infty)$, then

4. *$f * g \in C_0(\mathbb{R}^n)$.*

Let $p, q, r \in [1, \infty]$ satisfy $1/p + 1/q = 1 + 1/r$. If $f \in L^p(\mathbb{R}^n)$ and $g \in L^q(\mathbb{R}^n)$, then

5. *$f * g \in L^r(\mathbb{R}^n)$;*
6. *$\|f * g\|_{L^r(\mathbb{R}^n)} \leq \|f\|_{L^p(\mathbb{R}^n)} \|g\|_{L^q(\mathbb{R}^n)}$.*

Proof. The proof can be found in [11], p. 241. □

Statement 6 of Lemma 4.1 is called Young's inequality. It also holds for the convolution in time with upper bound t, which will appear in (18). This is shown in the following corollary:

Corollary 4.2. *Let T be fixed and let $p, q, r \in [1, \infty]$ satisfy $1/p + 1/q = 1 + 1/r$. If $f \in L^p([0, T])$ and $g \in L^q([0, T])$, then*

1. *$f *_t g := t \mapsto \int_0^t f(t - s)g(s)\, ds \in L^r([0, T])$;*
2. *$\|f *_t g\|_{L^r([0,T])} \leq \|f\|_{L^p([0,T])} \|g\|_{L^q([0,T])}$.*

Proof. The statement of this corollary follows from extension to $\mathbb{R}$ of f and g by zero outside $[0, T]$ and applying Lemma 4.1, Parts 5 and 6 (for $n = 1$). □

The Green's function of the diffusion operator on $\mathbb{R}^n$ is (for general dimension n) given by

$$G_t(x) := (4\pi dt)^{-n/2} \mathrm{e}^{-|x|^2/4dt}. \tag{7}$$

Lemma 4.3 (Properties of the Green's function on $\mathbb{R}^2$)**.** *Consider the Green's function (7) for dimension $n = 2$.*

1. *The gradient of the Green's function satisfies*

$$\|\nabla G_{\cdot}(x)\|_{L^\infty(0,\infty)} := \sup_{\tau \in (0,\infty)} \|\nabla G_\tau(x)\| = \begin{cases} 0, & x = 0; \\ \dfrac{8\mathrm{e}^{-2}}{\pi}\, |x|^{-3}, & x \in \mathbb{R}^2 \setminus \{0\}. \end{cases} \tag{8}$$

2. *For all $1 \leq p \leq \infty$ there is a constant c such that for all $t \in \mathbb{R}^+$*

$$\|G_t(\cdot)\|_{L^p(\mathbb{R}^2)} \leq c\, t^{\frac{1}{p}-1}. \tag{9}$$

The constant depends on p and d.

Proof.   1. For all $x \in \mathbb{R}^2$ and all $\tau \in \mathbb{R}^+$

$$\|\nabla G_\tau(x)\| = \frac{|x|}{8\pi d^2 \tau^2} \, \mathrm{e}^{-|x|^2/4d\tau}, \tag{10}$$

where $\| \cdot \|$ denotes the Euclidean norm on $\mathbb{R}^2$. For $x = 0$ we have that $\|\nabla G_\tau(0)\| = 0$ for all $\tau \in (0, \infty)$, thus the corresponding part of (8) follows.

Next, we consider $x \neq 0$. Note that for all such x

$$\lim_{\tau \to 0} \|\nabla G_\tau(x)\| = 0, \tag{11}$$

$$\lim_{\tau \to \infty} \|\nabla G_\tau(x)\| = 0. \tag{12}$$

Since the right-hand side in (10) is nonnegative and differentiable for all $\tau \in \mathbb{R}^+$, its maximum on $\mathbb{R}^+$ is attained where

$$\frac{\partial}{\partial \tau} \|\nabla G_\tau(x)\| = \frac{|x|}{4\pi d^2 \tau^3} \left(\frac{|x|^2}{8d\tau} - 1 \right) \mathrm{e}^{-|x|^2/4d\tau} = 0, \tag{13}$$

i.e. at $\tau = |x|^2/8d$. Now the statement of the lemma follows:

$$\|\nabla G_.(x)\|_{L^\infty(0,\infty)} = \|\nabla G_\tau(x)\| \Big|_{\tau = |x|^2/8d} = \frac{8\mathrm{e}^{-2}}{\pi} \, |x|^{-3}. \tag{14}$$

2. The proof is a direct consequence of the statement in [14] at the bottom of p. 432.

$\square$

5. **Solution concepts and their regularity.** For problem (1) we follow [8, 9] by considering solutions in the sense of $L^2(\Omega)$-valued distributions on $[0, T]$. Our setting is a special case of the setting in [9]. However, [9] is one of the few works that we are aware of that consider maximal regularity issues for problems in *unbounded* domains. The seminal works by Solonnikov [31] and Lasiecka [20] cover bounded domains Ω only.

We reformulate Theorem 2.1 in [9] to obtain:

Theorem 5.1. *If*

- $\phi \in H^1([0, T]; L^2(\Gamma)) \cap L^2([0, T]; H^1(\Gamma))$, *and*
- $u_0 \in H^1(\Omega)$,

then Problem (1) *has a unique solution*

$$u \in H^1([0, T]; L^2(\Omega)) \cap L^2([0, T]; H^2(\Omega)). \tag{15}$$

Proof. The statement of this theorem is fully covered by Theorem 2.1 in [9]. We now point out why we satisfy their conditions. Note that we use $p = 2$ and $m = 1$ in their setting. First, $\mathbb{R}$ is a so-called $\mathcal{HT}$-space, meaning that the Hilbert transform defines a bounded operator on $L^p(\mathbb{R})$ for $1 < p < \infty$ (cf. [28], VII). The conditions (E), (LS), (SD) and (SB) from [9] are easily verified for $\mathcal{A}u := -d\Delta u$ and $\mathcal{B}u := \nabla u \cdot n$. Regarding Condition (D) in [9], we note that in our case $f \equiv 0$ and moreover, no compatibility condition (iv) is needed. In (iii), we use that $B^1_{2,2}(\Omega) = H^1(\Omega)$; see [1] p. 231. A sufficient condition for (ii) to hold, is the one on ϕ given in the hypotheses of this theorem. We avoid the – in our setting unnecessary – use of fractional Sobolev spaces. $\square$

Problem (3) has a measure-valued right-hand side. [4] provide regularity results for weak solutions of non-linear parabolic problems with such measure-valued right-hand side. These apply to *bounded* domains with Dirichlet boundary condition and zero initial value.

We consider *mild solutions* to (3) in the Banach space of finite Borel measures on $\mathbb{R}^2$, completed for the dual bounded Lipschitz norm $\| \cdot \|_{\mathrm{BL}}^*$ or Fortet-Mourier norm: $\overline{\mathcal{M}}(\mathbb{R}^2)_{\mathrm{BL}}$ (cf. [15] and references found there). First, the diffusion semigroup $(S_t)_{t \geq 0}$ on $\overline{\mathcal{M}}(\mathbb{R}^2)_{\mathrm{BL}}$ is defined for measures $\mu \in \mathcal{M}(\mathbb{R}^2)$ by convolution with the Green's function G_t defined by (7), i.e.

$$\langle S_t \mu, \varphi \rangle := \langle G_t * \mu, \varphi \rangle = \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} G_t(x - y) \varphi(x) \, d\mu(y) \, dx \tag{16}$$

for $\varphi \in C_b(\mathbb{R}^2)$. Thus, for positive μ, $S_t \mu$ defines a positive linear functional on $C_c(\mathbb{R}^2)$, which is represented by a unique Radon measure according to the Riesz Representation Theorem. It is a finite measure because

$$(S_t \mu)(\mathbb{R}^2) = \langle S_t \mu, \mathbf{1} \rangle = \mu(\mathbb{R}^2) < \infty.$$

Using the Jordan decomposition, we see that $S_t \mu \in \mathcal{M}(\mathbb{R}^2)$ for any $\mu \in \mathcal{M}(\mathbb{R}^2)$. One can check using (16) that S_t is a bounded operator on $\mathcal{M}(\mathbb{R}^2)$ for $\| \cdot \|_{\mathrm{BL}}^*$. By continuity it extends to the completion $\overline{\mathcal{M}}(\mathbb{R}^2)_{\mathrm{BL}}$. Moreover, there exists $C > 0$ such that

$$\|S_t \nu\|_{\mathrm{BL}}^* \leq C \|\nu\|_{\mathrm{BL}}^*$$

for all $t \geq 0$ and $\nu \in \overline{\mathcal{M}}(\mathbb{R}^2)_{\mathrm{BL}}$. Strong continuity of $(S_t)_{t \geq 0}$ on $\overline{\mathcal{M}}(\mathbb{R}^2)_{\mathrm{BL}}$ can then be obtained from strong continuity on the dense subspace $\mathcal{M}(\mathbb{R}^2)$ that follows from (16) and [10], Proposition I.5.3.

The mild solution to (3) is now defined by

$$\hat{\mu}(t) := S(t)\mu_0 + \int_0^t S(t - s)[\bar{\phi}(s)\delta_0] \, ds, \tag{17}$$

for given initial measure $\mu_0 \in \mathcal{M}(\mathbb{R}^2)$ ([26], Ch.4, Def. 2.3, p.106). One can show that $\hat{\mu} \in C(\mathbb{R}_+, \overline{\mathcal{M}}(\mathbb{R}^2)_{\mathrm{BL}})$ whenever $\bar{\phi} \in L_{\mathrm{loc}}^1(\mathbb{R}_+)$.

If μ_0 has density $\hat{u}_0$ with respect to Lebesgue measure dx on $\mathbb{R}^2$, then according to (16) solution $\hat{\mu}(t)$ can be identified with $\hat{u}(x, t)dx$ where the density function $\hat{u}$ is given by

$$\hat{u}(x, t) = \int_{\mathbb{R}^2} G_t(x - y)\hat{u}_0(y) \, dy + \int_0^t G_{t-s}(x)\bar{\phi}(s) \, ds$$
$$=: (G_t *_x \hat{u}_0)(x) + (G_{\cdot}(x) *_t \bar{\phi})(t). \tag{18}$$

for all $(x, t) \in \mathbb{R}^2 \times \mathbb{R}^+$. Here the notation $*_x$ and $*_t$ emphasizes that one takes convolution with respect to the space or time variable. Both have a regularising effect on the solution, that yields the following result for the restriction of $\hat{u}(t)$ to Ω, the domain on which we compare with solution $u(t)$ to Problem (1):

Theorem 5.2. *If $\hat{u}_0 \in H^1(\mathbb{R}^2)$ and $\bar{\phi} \in H^1([0, T])$, then $\hat{u}$ (restricted to Ω) satisfies*

$$\hat{u} \in H^1([0, T]; L^2(\Omega)) \cap L^2([0, T]; H^2(\Omega)). \tag{19}$$

Moreover, $\partial_t \hat{u}(t) = d\Delta \hat{u}(t)$ in $L^2(\Omega)$ for almost every t in $[0, T]$.

Proof. See Appendix.   □

6. **Flux estimates.** In this section we present in Theorem 6.3 a bound on the difference between the fluxes on Γ in (1) and (3). According to Theorem 5.1 and Theorem 5.2, under the conditions for which these results hold, $c^*(t)$ defined by (4) is finite for every $t \in [0, T]$. The difference between the solutions u and $\hat{u}$ on Ω will be expressed in terms of $c^*(t)$, among others, in Section 7.

Throughout this section, we shall assume the conditions of Theorems 5.1 and 5.2 on the data. Note that $\bar{\phi} \in H^1([0,T])$ implies that

$$\int_0^t \|\bar{\phi}\|_{L^1(0,\tau)}^2 \, d\tau \leq \tfrac{1}{2}t^2 \|\bar{\phi}\|_{L^2([0,T])}^2 < \infty \tag{20}$$

for all $0 \leq t \leq T$.

Before getting at the main estimate for $c^*(t)$, we derive auxiliary results in Lemma 6.1 and Lemma 6.2.

Lemma 6.1. *Assume that $\hat{u}_0 \equiv 0$. Then, for all $t > 0$ we have*

$$\int_0^t \|d\nabla \hat{u} \cdot n\|_{L^2(\Gamma)}^2 \leq d^2 C_\Gamma \int_0^t \|\bar{\phi}\|_{L^1(0,\tau)}^2 \, d\tau < \infty, \tag{21}$$

where

$$C_\Gamma := \int_\Gamma \|\nabla G.(x)\|_{L^\infty(0,\infty)}^2 \, d\sigma > 0$$

is independent of t.

Proof. For $\hat{u}_0 \equiv 0$, the solution (18) of (3) is given by

$$\hat{u}(x,t) = \int_0^t G_{t-s}(x)\bar{\phi}(s) \, ds. \tag{22}$$

Note that for $x \in \Gamma$ we have

$$\begin{aligned}
|d\nabla \hat{u}(x,\tau) \cdot n(x)| &= \left| d \int_0^\tau \nabla G_{\tau-s}(x)\bar{\phi}(s) \, ds \cdot n(x) \right| \\
&\leq \left\| d \int_0^\tau \nabla G_{\tau-s}(x)\bar{\phi}(s) \, ds \right\| \\
&\leq d \|\nabla G.(x)\|_{L^\infty(0,\infty)} \int_0^\tau |\bar{\phi}(s)| \, ds \\
&= d \|\nabla G.(x)\|_{L^\infty(0,\infty)} \|\bar{\phi}\|_{L^1(0,\tau)}. \tag{23}
\end{aligned}$$

We emphasize here that the infinity norm $\|\nabla G.(x)\|_{L^\infty(0,\infty)}$ denotes the supremum in the time domain for fixed x, cf. (8). This observation leads to the following estimate

$$\begin{aligned}
\int_0^t \|d\nabla \hat{u}(x,\tau) \cdot n(x)\|_{L^2(\Gamma)}^2 \, d\tau &= \int_0^t \int_\Gamma |d\nabla \hat{u}(x,\tau) \cdot n(x)|^2 \, d\sigma \, d\tau \\
&\leq d^2 \int_0^t \int_\Gamma \|\nabla G.(x)\|_{L^\infty(0,\infty)}^2 \|\bar{\phi}\|_{L^1(0,\tau)}^2 \, d\sigma \, d\tau, \tag{24}
\end{aligned}$$

where (23) is used in the second step. Thus, we have

$$\int_0^t \|d\nabla \hat{u}(x,\tau) \cdot n(x)\|_{L^2(\Gamma)}^2 \, d\tau \leq d^2 \int_0^t \|\bar{\phi}\|_{L^1(0,\tau)}^2 d\tau \int_\Gamma \|\nabla G.(x)\|_{L^\infty(0,\infty)}^2 \, d\sigma. \tag{25}$$

Since Γ has finite length and it is the boundary of a set of which 0 is an interior point, it follows from (8) in Lemma 4.3 that the second integral on the right-hand side of (25) is finite. This finishes the proof. $\square$

In the next lemma we generalize this result to nonzero initial conditions.

Lemma 6.2. *If $\hat{u}_0$ is such that $\nabla\hat{u}_0 \in L^p(\mathbb{R}^2)$ for some $2 < p \leq \infty$, then*

$$\int_0^t \|d\nabla\hat{u} \cdot n\|_{L^2(\Gamma)}^2 \leq d^2|\Gamma|Ct^{\frac{2}{q}-1}\|\nabla\hat{u}_0\|_{L^p(\mathbb{R}^2)}^2 + 2d^2C_\Gamma \int_0^t \|\bar{\phi}\|_{L^1(0,\tau)}^2 \, d\tau < \infty, \quad (26)$$

for all $t > 0$, where $q := p/(p-1)$, C depends on d and q and C_Γ is the constant from Lemma 6.1.

Proof. In this case, the solution of (3) is given by (18). We start with the following estimate

$$\int_0^t \|d\nabla\hat{u}(x,\tau) \cdot n(x)\|_{L^2(\Gamma)}^2 \, d\tau \leq 2 \int_0^t \int_\Gamma \left| d\nabla \int_{\mathbb{R}^2} G_\tau(x-y)\hat{u}_0(y) \, dy \cdot n(x) \right|^2 \, d\sigma \, d\tau$$

$$+ 2 \int_0^t \int_\Gamma \left| d\nabla \int_0^\tau G_{\tau-s}(x)\bar{\phi}(s) \, ds \cdot n(x) \right|^2 \, d\sigma \, d\tau. \quad (27)$$

The second term on the right-hand side is covered by Lemma 6.1. Regarding the first term, we remark that, due to properties of the convolution,

$$\left| d\nabla \int_{\mathbb{R}^2} G_\tau(x-y)\hat{u}_0(y) \, dy \cdot n(x) \right| = \left| d \int_{\mathbb{R}^2} G_\tau(y)\nabla\hat{u}_0(x-y) \, dy \cdot n(x) \right|. \quad (28)$$

We use Part 3 of Lemma 4.1 to estimate the right-hand side

$$\left| d \int_{\mathbb{R}^2} G_\tau(y)\nabla\hat{u}_0(x-y) \, dy \cdot n(x) \right| \leq d \left\| \int_{\mathbb{R}^2} G_\tau(y)\nabla\hat{u}_0(\cdot - y) \, dy \right\|_{L^\infty(\mathbb{R}^2)}$$

$$\leq d \, \|\nabla\hat{u}_0\|_{L^p(\mathbb{R}^2)} \, \|G_\tau\|_{L^q(\mathbb{R}^2)}, \quad (29)$$

with $q := p/(p-1)$.

It follows from (28)–(29) and Part 2 of Lemma 4.3 that

$$\int_0^t \int_\Gamma \left| d\nabla \int_{\mathbb{R}^2} G_\tau(x-y)\hat{u}_0(y) \, dy \cdot n(x) \right|^2 \, d\sigma \, d\tau$$

$$\leq d^2 \, \|\nabla\hat{u}_0\|_{L^p(\mathbb{R}^2)}^2 \int_0^t \int_\Gamma \|G_\tau\|_{L^q(\mathbb{R}^2)}^2 \, d\sigma \, d\tau$$

$$\leq c^2 \, d^2 \, |\Gamma| \, \|\nabla\hat{u}_0\|_{L^p(\mathbb{R}^2)}^2 \int_0^t \tau^{\frac{2}{q}-2} \, d\tau$$

$$= \frac{q \, c^2 \, d^2 \, |\Gamma|}{2-q} \, t^{\frac{2}{q}-1} \, \|\nabla\hat{u}_0\|_{L^p(\mathbb{R}^2)}^2, \quad (30)$$

where c depends on q and d. We can perform the integration in time in the last step of (30) since the hypothesis $p > 2$ implies $q < 2$. The desired result follows by (27) and the calculations in the proof of Lemma 6.1:

$$\int_0^t \|d\nabla\hat{u}(x,\tau) \cdot n(x)\|_{L^2(\Gamma)}^2 \, d\tau \leq \frac{2q \, c^2 \, d^2 \, |\Gamma|}{2-q} \, t^{\frac{2}{q}-1} \, \|\nabla\hat{u}_0\|_{L^p(\mathbb{R}^2)}^2$$

$$+ 2d^2 \int_0^t \|\bar{\phi}\|_{L^1(0,\tau)}^2 d\tau \int_\Gamma \|\nabla G.(x)\|_{L^\infty(0,\infty)}^2 \, d\sigma, \quad (31)$$

of which the right-hand side is finite for all finite t. $\square$

Remark 5. A sufficient condition for $\nabla\hat{u}_0 \in L^p(\mathbb{R}^2)$ to hold, is $\hat{u}_0 \in W^{1,p}(\mathbb{R}^2)$. To this aim, one may start from $u_0 \in W^{1,p}(\Omega)$ to hold for the *given* initial data. The remaining question is whether it is possible to find an extension v_0 on $\Omega_\mathcal{O}$ as in (2)

such that $\hat{u}_0 \in W^{1,p}(\mathbb{R}^2)$. This, however is guaranteed by Theorem 5.22 on p. 151 of [1].

Remark 6. It is crucial that the gradient is applied to the initial condition in the computations starting at (28) and further. Instead of (28)–(29), we could, along the same lines, have estimated

$$\left| d\,\nabla \int_{\mathbb{R}^2} G_\tau(x - y)\hat{u}_0(y)\,dy \cdot n(x) \right| \leq d\,\|\hat{u}_0\|_{L^p(\mathbb{R}^2)}\,\|\nabla G_\tau\|_{L^q(\mathbb{R}^2)}\,, \qquad (32)$$

which requires only a condition on $\hat{u}_0$, not on its gradient, for the lemma. It follows from [14] (p. 432, bottom) that for some constant C

$$\|\nabla G_\tau\|_{L^q(\mathbb{R}^2)} \leq C\,\tau^{\frac{1}{q} - \frac{3}{2}}. \qquad (33)$$

This is a problem however, since similar arguments as in (30) would lead to

$$\int_0^t \|\nabla G_\tau\|_{L^q(\mathbb{R}^2)}^2 \, d\tau \leq C \int_0^t \tau^{\frac{2}{q} - 3} \, d\tau, \qquad (34)$$

of which the right-hand side is not integrable for any $1 \leq q \leq \infty$.

We now come to the summarizing result of this section.

Theorem 6.3. *Assume that the hypotheses of Theorems* 5.1 *and* 5.2 *and Lemma* 6.2 *hold. Then, for all $t > 0$ the function c^* defined by* (4) *satisfies*

$$c^*(t) \leq 2 \int_0^t \|\phi\|_{L^2(\Gamma)}^2 + 2d^2|\Gamma|Ct^{\frac{2}{q} - 1}\|\nabla\hat{u}_0\|_{L^p(\mathbb{R}^2)}^2 + 2C_\Gamma \int_0^t \|\bar{\phi}\|_{L^1(0,\tau)}^2 \, d\tau. \qquad (35)$$

Proof. The statement of this theorem is a direct consequence of the observation

$$\int_0^t \|\phi - d\nabla\hat{u} \cdot n\|_{L^2(\Gamma)}^2 \leq 2 \int_0^t \|\phi\|_{L^2(\Gamma)}^2 + 2 \int_0^t \|d\nabla\hat{u} \cdot n\|_{L^2(\Gamma)}^2. \qquad (36)$$

The first term is finite due to the assumption that $\phi \in L^2([0, T]; L^2(\Gamma))$ for all $T \in \mathbb{R}^+$ (see Section 2). The second term was estimated in Lemma 6.2. $\qquad \square$

Remark 7. Estimate (35) is unsatisfactory for t close to zero. However, it shows for large t that on the long run the difference between the fluxes on Γ is dominated by the prescribed fluxes ϕ at Γ and $\bar{\phi}$ at the point source at 0, rather than the initial condition, which is clear intuitively. In Section 8 we provide a further discussion of the behaviour of $c^*(t)$.

7. **Estimates in the exterior – Proof of Theorem 3.1.** We can now prove our main result, an estimate for the difference between the solutions u of (1) and $\hat{u}$ of (3) (using the solution concept explained in Section 5):

Proof. (Theorem 3.1). Let $\psi \in C_c^\infty(\overline{\Omega})$ and $h \in C_c^\infty([0, T])$ be test functions. Put $(\psi \otimes h)(x, t) := \psi(x)h(t)$. Then according to Theorem 5.1 and Theorem 5.2 one has

$$\langle \partial_t u - \partial_t \hat{u}, \psi \otimes h \rangle = d\,\langle \Delta u - \Delta \hat{u}, \psi \otimes h \rangle$$

$$= \int_0^T \left\{ \int_\Gamma (\phi(t) - d\nabla\hat{u}(t) \cdot n)\,\psi \right\} h(t)dt \qquad (37)$$

$$- d \int_0^T \left\{ \int_\Omega (\nabla u - \nabla\hat{u}) \cdot \nabla\psi \right\} h(t)dt.$$

Because of the regularity of the solutions u and $\hat{u}$ identity (37) extends to functions $f \in L^1([0,T], H^1(\Omega))$ by continuity:

$$\langle \partial_t u - \partial_t \hat{u}, f \rangle = \int_0^T \int_\Gamma (\phi(t) - d\nabla\hat{u}(t) \cdot n) \, f(x,t) \, d\sigma(x) \, dt$$
$$- d \int_0^T \int_\Omega (\nabla u - \nabla\hat{u}) \cdot \nabla f(x,t) \, dx \, dt. \tag{38}$$

Now take $f(x,t) := (u(x,t) - \hat{u}(x,t))h(t)$ with $h \in C_c^\infty([0,T])$ arbitrary. Then the regularity of u and $\hat{u}$ and (38) imply that

$$\frac{1}{2}\frac{d}{dt}\|u - \hat{u}\|_{L^2(\Omega)}^2 + d\|\nabla u - \nabla\hat{u}\|_{L^2(\Omega)}^2 = \int_\Gamma (u - \hat{u})(\phi - d\nabla\hat{u}\cdot n) \,. \tag{39}$$

Add $d\|u - \hat{u}\|_{L^2(\Omega)}^2$ to both sides and integrate in time from 0 to arbitrary t:

$$\frac{1}{2}\|u - \hat{u}\|_{L^2(\Omega)}^2 + d\int_0^t \|u - \hat{u}\|_{H^1(\Omega)}^2 = \int_0^t \int_\Gamma (u - \hat{u})(\phi - d\nabla\hat{u}\cdot n) \ + d\int_0^t \|u - \hat{u}\|_{L^2(\Omega)}^2 \,, \tag{40}$$

where we have used that u and $\hat{u}$ are initially equal on Ω. Apply the Cauchy-Schwarz inequality and use the result of Theorem 6.3 to obtain

$$\int_0^t \int_\Gamma (u - \hat{u})(\phi - d\nabla\hat{u}\cdot n) \ \leq \left(\int_0^t \|u - \hat{u}\|_{L^2(\Gamma)}^2 \right)^{\frac{1}{2}} \left(\int_0^t \|\phi - d\nabla\hat{u}\cdot n\|_{L^2(\Gamma)}^2 \right)^{\frac{1}{2}}$$
$$= \sqrt{c^*(t)} \left(\int_0^t \|u - \hat{u}\|_{L^2(\Gamma)}^2 \right)^{\frac{1}{2}} \,. \tag{41}$$

Since $H^1(\Omega) \hookrightarrow L^2(\Gamma)$, according to the Boundary Trace Imbedding Theorem (cf. [1], Theorem 5.36, p. 164) there is a constant $\bar{c} = \bar{c}(\Omega) > 0$ such that

$$\|u - \hat{u}\|_{L^2(\Gamma)} \leq \bar{c}\|u - \hat{u}\|_{H^1(\Omega)}, \tag{42}$$

which can be used to further estimate (41):

$$\int_0^t \int_\Gamma (u - \hat{u})(\phi - d\nabla\hat{u}\cdot n) \ \leq \sqrt{c^*(t)}\,\bar{c} \left(\int_0^t \|u - \hat{u}\|_{H^1(\Omega)}^2 \right)^{\frac{1}{2}} \,. \tag{43}$$

For arbitrary $\varepsilon > 0$, Young's inequality yields the following estimate on the right-hand side:

$$\sqrt{c^*(t)}\,\bar{c} \left(\int_0^t \|u - \hat{u}\|_{H^1(\Omega)}^2 \right)^{\frac{1}{2}} \leq \frac{1}{2\varepsilon}c^*(t)\bar{c}^2 + \frac{\varepsilon}{2}\int_0^t \|u - \hat{u}\|_{H^1(\Omega)}^2 \,. \tag{44}$$

Take $\varepsilon \in (0, 2d)$. Then (40)–(44) together yield

$$\|u - \hat{u}\|_{L^2(\Omega)}^2 + (2d - \varepsilon)\int_0^t \|u - \hat{u}\|_{H^1(\Omega)}^2 \leq \frac{1}{\varepsilon}c^*(t)\bar{c}^2 + 2d\int_0^t \|u - \hat{u}\|_{L^2(\Omega)}^2 \,, \tag{45}$$

or

$$\|u - \hat{u}\|_{L^2(\Omega)}^2 + \underbrace{(2d - \varepsilon)\int_0^t \|\nabla u - \nabla\hat{u}\|_{L^2(\Omega)}^2}_{\geq 0} \leq \frac{1}{\varepsilon}c^*(t)\bar{c}^2 + \varepsilon\int_0^t \|u - \hat{u}\|_{L^2(\Omega)}^2 \,. \tag{46}$$

It follows that

$$\|u - \hat{u}\|_{L^2(\Omega)}^2 \leq \frac{1}{\varepsilon}c^*(t)\bar{c}^2 + \varepsilon\int_0^t \|u - \hat{u}\|_{L^2(\Omega)}^2 \,, \tag{47}$$

and due to a version of Gronwall's lemma[1]

$$\|u - \hat{u}\|^2_{L^2(\Omega)} \leq \frac{1}{\varepsilon} c^*(t) \bar{c}^2 \, \mathrm{e}^{\varepsilon t}, \tag{48}$$

where we use that $c^*(\cdot)$ is (by definition) non-decreasing. Note that ε is arbitrary but fixed, thus $1/\varepsilon < \infty$. We obtain (5) by defining $c_1 := \bar{c}^2/\varepsilon$.

From (45) it also follows that

$$\int_0^t \|u - \hat{u}\|^2_{H^1(\Omega)} \leq \frac{1}{\varepsilon(2d - \varepsilon)} c^*(t) \bar{c}^2 + \frac{2d}{2d - \varepsilon} \int_0^t \|u - \hat{u}\|^2_{L^2(\Omega)} . \tag{49}$$

The upper bound (48) now implies

$$\int_0^t \|u - \hat{u}\|^2_{H^1(\Omega)} \leq \frac{1}{\varepsilon(2d - \varepsilon)} c^*(t) \bar{c}^2 + \frac{2d}{\varepsilon^2(2d - \varepsilon)} c^*(t) \bar{c}^2 \, (\mathrm{e}^{\varepsilon t} - 1)$$

$$\leq \frac{2d}{\varepsilon^2(2d - \varepsilon)} c^*(t) \bar{c}^2 \, \mathrm{e}^{\varepsilon t}, \tag{50}$$

where we use that $\varepsilon < 2d$ in the second step. The second statement of the theorem now follows by defining $c_2 := 2d\bar{c}^2/(\varepsilon^2(2d - \varepsilon))$. $\square$

Remark 8. In principle, (50) can be optimized in ε for every t separately, to get an optimal $\varepsilon = \varepsilon(t)$. After substitution of this $\varepsilon(t)$, (6) becomes independent of ε. However, its t-dependence obviously becomes more complicated. Further details on this aspect are omitted here.

Remark 9. The fact that the estimates in Theorem 3.1 are linear in c^* relates nicely to our Conjecture 1; see Section 8 below. If indeed c^* is small or even goes to zero, then the same holds for $\|u(\cdot, t) - \hat{u}(\cdot, t)\|^2_{L^2(\Omega)}$ and $\int_0^t \|u - \hat{u}\|^2_{H^1(\Omega)}$.

8. **Conjecture.** The estimate (36) is a very crude way to find an upper bound on $c^*(t)$. In the following (deliberately vague) conjecture, we express under which conditions we expect $c^*(t)$ to be smaller than the upper bound of Theorem 6.3 suggests.

Conjecture 1. *The upper bound c^* can be much smaller than Theorem 6.3 suggests. Ideally it goes to zero.*

Conjecture 1 is based on the following considerations:
- Once the geometry and ϕ on Γ are given, there still is a lot of freedom in dealing with the reduced problem (3). We can choose $\bar{\phi}$ and v_0. Our conjecture is that a smart choice of $\bar{\phi}$ and v_0 can produce a flux on Γ that mimics well ϕ and gives more than merely a *bounded* difference.
- Initially, during a small time interval, the initial condition should induce a sufficiently close flux. To this aim an appropriate v_0 has to be provided.
- At a certain moment, mass originating from the source starts reaching the boundary. From then onwards, the mimicking flux should be – with some delay – mainly due to $\bar{\phi}$.
- Let $|\Omega_{\mathcal{O}}|$ denote a typical length scale of the object $\mathcal{O}$ (e.g. its diameter). The quantity $|\Omega_{\mathcal{O}}|^2/d$ is a typical timescale for points to travel the distance from source to boundary. This is also the timescale at which the transition between the above two bullet points takes place.

---

[1]A specific form of Theorem 1 on p. 356 of [25].

- The shape of object $\mathcal{O}$ is important. An intuitive guess is that a small object $\mathcal{O}$ can be better approximated. As the point source emits mass at the same rate in all directions, we expect a better approximation also to be possible if Γ is radially symmetric with respect to the origin, and ϕ is constant on Γ (in space, not necessarily in time). A generalization of the latter condition would be to have ϕ defined on a more general Γ, but to have an extension to a ball $B(0, R)$ such that $\Gamma \subset B(0, R) \subset \mathbb{R}^2$, and this extension is radially symmetric around the origin on $B(0, R)$.

The above statement was written under the assumption that in general the (normal component of the) flux is directed outward on Γ. For a mass sink, *mutatis mutandis* the same considerations hold.

Appendix – Proof of Theorem 5.2.

Proof. Note that for $\hat{u}_0 \in H^1(\mathbb{R}^2)$, the function $\hat{u}_1 := G *_x \hat{u}_0$ is a solution of

$$
\begin{cases}
\dfrac{\partial u}{\partial t} = d\Delta u, & \text{on } \mathbb{R}^2 \times \mathbb{R}^+; \\
u(0) = \hat{u}_0, & \text{on } \mathbb{R}^2,
\end{cases}
\tag{51}
$$

which is unique and satisfies

$$
\hat{u}_1 \in H^1([0, T]; L^2(\mathbb{R}^2)) \cap L^2([0, T]; H^2(\mathbb{R}^2))
\tag{52}
$$

due to [9], Theorem 2.1, where the domain is taken to be $\mathbb{R}^2$.

Define $\hat{u}_2 := G *_t \bar{\phi}$. Then $\hat{u}_2$ satisfies

$$
\begin{aligned}
\|\hat{u}_2\|_{L^2(\Omega)} &= \left(\int_\Omega \left| \int_0^t G_{t-s}(x)\, \bar{\phi}(s)\, ds \right|^2 dx \right)^{1/2} \\
&\leq \int_0^t \left(\int_\Omega \left| G_{t-s}(x)\, \bar{\phi}(s) \right|^2 dx \right)^{1/2} ds \\
&\leq \int_0^t \|G_{t-s}\|_{L^2(\mathbb{R}^2)} |\bar{\phi}(s)|\, ds \\
&\leq \int_0^t c\, (t-s)^{-1/2} |\bar{\phi}(s)|\, ds.
\end{aligned}
\tag{53}
$$

In the second step we used Minkowski's inequality for integrals (see [32], p. 271), whereas the last inequality follows from Part 2 of Lemma 4.3. Since $t \mapsto c\, t^{-1/2} \in L^1([0, T])$ and by assumption $\bar{\phi} \in L^2([0, T])$, Corollary 4.2 applied to (53) yields

$$
\|\hat{u}_2\|_{L^2(\Omega)} \in L^2([0, T]).
\tag{54}
$$

Because $G_.(x)$ and $\partial_t G_.(x)$ are in $L^1_{\text{loc}}(\mathbb{R}_+)$ for $x \neq 0$ and $\partial_t \bar{\phi} \in L^2(\mathbb{R}_+)$, one has in the sense of distributions

$$
\partial_t \big(G_.(x) * \bar{\phi} \big) = \big(\partial_t G_.(x) \big) * \bar{\phi} = G_.(x) * \big(\partial_t \bar{\phi} \big).
\tag{55}
$$

Thus we can repeat the argument leading to (54), replacing $\bar{\phi}$ by $\partial_t \bar{\phi}$, and obtain

$$\|\partial_t \hat{u}_2\|_{L^2(\Omega)} \in L^2([0, T]). \tag{56}$$

We conclude from (54) and (56) that

$$\hat{u}_2 \in H^1([0, T]; L^2(\Omega)). \tag{57}$$

It follows from (7), with $n = 2$ that

$$\partial_{x_i} G_t(x) = \frac{x_i}{8\pi d^2 t^2} e^{-|x|^2/4dt}, \text{ and} \tag{58}$$

$$\partial_{x_i} \partial_{x_j} G_t(x) = \frac{1}{8\pi d^2 t^2} e^{-|x|^2/4dt} \left[\delta_{ij} - \frac{x_i x_j}{2dt} \right], \tag{59}$$

where δ_{ij} denotes the Kronecker delta. The gradient is bounded in the following way:

$$|\nabla G_t(x)|^2 \leq \sup_{t>0} |\nabla G_t(x)|^2$$

$$= \sup_{t>0} \frac{|x|^2}{64\pi^2 d^4 t^4} e^{-|x|^2/2dt}$$

$$= \frac{1}{|x|^6} \sup_{u>0} \frac{u^4}{4\pi^2} e^{-u}, \tag{60}$$

for all $t > 0$ and for all $x \in \Omega$, where we substituted $u := |x|^2/2dt$ to obtain the constant $c_1 := \sup_{u>0} \frac{u^4}{4\pi^2} e^{-u}$, which is independent of $|x|$, t, d. Thus

$$|\nabla G_t(x)|^2 \leq \frac{c_1}{|x|^6}. \tag{61}$$

For a matrix $M \in \mathbb{R}^{n \times n}$, as matrix norm we use the Frobenius norm and denote it by $\| \cdot \|_F$:

$$\|M\|_F := \sqrt{\sum_{i,j} |M_{ij}|^2}. \tag{62}$$

In a similar way as for ∇G, we estimate the Hessian matrix

$$\|D^2 G_t(x)\|_F^2 \leq \sup_{t>0} \left(\sum_{i=1}^{2} \sum_{j=1}^{2} \frac{1}{64\pi^2 d^4 t^4} e^{-|x|^2/2dt} \left[\delta_{ij} - \frac{x_i x_j}{2dt} \right]^2 \right)$$

$$= \sup_{t>0} \frac{1}{64\pi^2 d^4 t^4} e^{-|x|^2/2dt} \left(2 - \frac{|x|^2}{dt} + \frac{|x|^4}{4d^2 t^2} \right)$$

$$= \frac{1}{|x|^8} \sup_{u>0} \frac{u^4}{4\pi^2} e^{-u} \left(2 - 2u + u^2 \right)$$

$$= \frac{c_2}{|x|^8}, \tag{63}$$

for all $t > 0$ and for all $x \in \Omega$. Now we show that $\partial_{x_i} G_t$ and $\partial_{x_i} \partial_{x_j} G_t$ are in $L^2(\Omega)$, both with uniform upper bound in t:

$$\|\partial_{x_i} G_t\|_{L^2(\Omega)}^2 = \int_\Omega |\partial_{x_i} G_t(x)|^2 \, dx$$

$$\leq \int_\Omega |\nabla G_t(x)|^2 \, dx$$

$$\overset{(61)}{\leq} \int_\Omega \frac{c_1}{|x|^6}\, dx =: C_1 < \infty, \tag{64}$$

where we use that 0 is an interior point of $\Omega_{\mathcal{O}} = \mathbb{R}^2 \setminus \overline{\Omega}$. Also

$$\|\partial_{x_i}\partial_{x_j}G_t\|^2_{L^2(\Omega)} = \int_\Omega |\partial_{x_i}\partial_{x_j}G_t(x)|^2\, dx$$

$$\leq \int_\Omega \|D^2 G_t(x)\|^2_F\, dx$$

$$\overset{(63)}{\leq} \int_\Omega \frac{c_2}{|x|^8}\, dx =: C_2 < \infty. \tag{65}$$

For brevity, we now use the index notation for derivatives and, for $|\alpha| \in \{1, 2\}$. Like in (53), using Minkowski's integral inequality, we obtain that

$$\|\partial_x^\alpha \hat{u}_2\|_{L^2(\Omega)} \leq \int_0^t \|\partial_x^\alpha G_{t-s}\|_{L^2(\Omega)} |\bar{\phi}(s)|\, ds. \tag{66}$$

Due to (64)–(65), for each $|\alpha| \in \{1, 2\}$ and for each $\tau > 0$

$$\|\partial_x^\alpha G_\tau\|_{L^2(\Omega)} \in L^\infty([0, T]) \subset L^1([0, T]). \tag{67}$$

Hence, the fact that $\bar{\phi} \in L^2([0, T])$ yields via Part 2 of Corollary 4.2 that

$$\int_0^t \|\partial_x^\alpha G_{t-s}\|_{L^2(\Omega)} |\bar{\phi}(s)|\, ds \in L^2([0, T]), \tag{68}$$

for each $|\alpha| \in \{1, 2\}$. It follows from (54), (66) and (68) that

$$\hat{u}_2 \in L^2([0, T]; H^2(\Omega)). \tag{69}$$

Together with (57), this finishes the proof of the first part.

The last statement follows from (55) and a similar result for the spatial derivatives. For all $\psi \in C_c^\infty(\overline{\Omega})$ and $h \in C_c^\infty(\mathbb{R}_+)$, $\psi \otimes h(x, t) := \psi(x)h(t)$ is in $C_c^\infty(\overline{\Omega} \times \mathbb{R}_+)$ and one has

$$\langle \partial_t \hat{u}, \psi \otimes h \rangle = \big\langle (\partial_t G.) *_x \hat{u}_0, \psi \otimes h \big\rangle + \int_{\overline{\Omega}} \big\langle \partial_t [G.(x)] *_t \bar{\phi}, h \big\rangle \psi(x)\, dx$$

$$= \langle d(\Delta G.) *_x \hat{u}_0, \psi \otimes h \rangle + \int_{\overline{\Omega}} \big\langle d[\Delta G.(x)] *_t \bar{\phi}, h \big\rangle \psi(x)\, dx$$

$$= \langle d\Delta(G. *_x \hat{u}_0), \psi \otimes h \rangle + \big\langle d\Delta(G. *_t \bar{\phi}), \psi \otimes h \big\rangle$$

$$= \langle d\Delta \hat{u}, \psi \otimes h \rangle.$$

By density of $C_c^\infty(\overline{\Omega}) \otimes C_c^\infty(\mathbb{R}_+)$ in the space of test functions $\mathcal{D}(\overline{\Omega} \times \mathbb{R}_+)$ we obtain $\partial_t \hat{u} = d\Delta \hat{u}$ in the sense of distributions on $\overline{\Omega} \times \mathbb{R}_+$. Since both are given by (locally integrable) functions according to the first part of the proof, $\partial_t \hat{u}(t) = d\Delta \hat{u}(t)$ for almost every t. $\qquad\square$

Remark 10. The estimates (64)–(65) hinge on the fact that Ω is bounded away from 0, where the integrand is singular.

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