Abstract—We consider the problem of characterizing the first arrival position (FAP) density in molecular communication (MC) with a diffusion-advection channel that permits a constant drift velocity pointed to arbitrary direction. The advantage of FAP modulation lies in the fact that it could encode more information into higher dimensional spatial variables, compared to other modulation techniques using time or molecule numbers. However, effective methods to characterize the FAP density in a general framework do not exist. In this paper, we devise a methodology that fully resolves the FAP density with planar absorbing receivers in arbitrary dimensions. Our work recovers existing results of FAP in 2D and 3D as special cases. The key insight of our approach is to remove the time dependence of the MC system evolution based on the generator of diffusion semigroups.

Index Terms—Molecular communication, diffusion, first arrival time (FAT), first arrival position (FAP), semigroup, generator.

I. INTRODUCTION

Since ancient times, the problem of conveying information over a distance has been an important issue in human history. Modern communication systems resolve this problem with electromagnetic (EM) signals. However, EM-based communication techniques are challenging for tiny (for instance, nanoscale) devices; if not feasible, due to the constraints such as the wavelength, antenna size, or energy issues [1], [2].

In molecular communication (MC) systems, small molecules called message molecules (MMs) act as chemical signals conveying the information [3], [4]. After the information-carrying particles are released in the channel, a propagation mechanism is necessary for transporting them to the receiver. This mechanism can be diffusion-based [5], flow-based [6], or an engineered transport system such as molecular motors [7], [8]. Among these different propagation mechanisms, diffusion-based MC, sometimes in combination with advection and chemical reaction networks, has been the most prevalent approach for MC systems, and will be the main focus of study in this paper.

In order to transmit information in a diffusion-based MC system, we can modulate different physical properties of the MMs [9], [12]. Signaling molecules that reach the vicinity of the receiver can be observed and processed by the receiver to extract the information that is necessary for performing detection and decoding [13]. The reception mechanism of a MC receiver can be categorized into two classes: i) passive reception, and ii) active reception. The simplest active reception is the fully-absorbing receiver [14] which has the ability to measure the time and position of arrival of each molecule, and to remove the MM right after it is received. For MC systems with a fully-absorbing receiver, how to completely characterize the arrival time or the arrival position is no doubt a very important issue.

In Section II-A we briefly review some important results concerning first arrival time (FAT) in MC literature. Until very recently, the first arrival position (FAP) information was also introduced into the MC realm, see [15], [16]. We will give a short introduction to the current status of FAP results in Section II-B.

A. First Arrival Time

When information is encoded on the time of release of MM, we refer to this subclass of MC channels as molecular timing channels (MTCs). The main difference between timing-based modulation and other modulations, such as the number or type modulation, is that: the channel input is continuous instead of discrete.

The MTC model was first proposed in [17]. In its simplest form, a MTC can be realized through a single MM released by the transmitter (Tx) at time $t_{in}$ with information encoded on this release time. The MM goes through some random propagation and arrive at the receiver (Rx) at time $t_{out}$. We have

$$t_{out} = t_{in} + t_{n},$$

(1)

where $t_{n}$ is some random delay due to MM propagation mechanisms. Unlike other modulation techniques, which typically permit finite alphabet, the symbol set of $t_{in}$ can be a continuous interval. It is worth pointing out that Eq. (1) can be regarded as an additive time invariant channel (with $t_{in}$ being the channel input and $t_{out}$ being the output) if the distribution of the random delay $t_{n}$ is stationary.

For MTC models that can be described by Eq. (1), the probability distribution of the random delay $t_{n}$ fully characterized the channel property. Considering a 1D environment with
an absorbing receiver, this random delay is Levy distributed [18] for free diffusion, and inverse Gaussian distributed for diffusion with drift [19]. A 3D vessel-like environment with drift can be approximated as a 1D environment [20], so the same distributions can be utilized for such environments under suitable conditions.

After the FAT density was introduced, timing-based techniques were further explored to understand the fundamental limits of MTCs. In [21], an MTC with additive inverse Gaussian noise (AIGN) was introduced, where \( t_n \) in Eq. (1) is inverse Gaussian distributed. The authors of [21] derived upper and lower bounds on capacity per channel use. Later in [19], tighter bounds on capacity of the same MTC with AIGN noise were derived. The capacity-achieving MM input distribution was also characterized. In [22]–[24], single particle release is extended to multiple, say \( M \) MM releases. In this scenario, information is encoded in a vector \( \mathbf{t} \), in which each component is the time of release of one of the \( M \) MMNs. For multiple particle case, the channel model changes to:

\[
t_{\text{out}} = \text{sort}(t_{\text{in}} + t_n),
\]

where \( t_n \) is an \( \mathbb{R}^M \) vector of random delays associated with each MM. Notice that \( \text{sort}(\mathbf{t}) \) is the sort operator that permutes the input vector into an ascending order. The sort operation is necessary when time information of each MM is considered since the MMNs may arrive out of order.

**B. First Arrival Position**

Apart from the first arrival time, there is another important degree of freedom to carry information: the first arrival position. The simplest FAP channel can be written as

\[
x_{\text{out}} = x_{\text{in}} + x_n,
\]

where \( x_{\text{in}}, x_{\text{out}} \) and \( x_n \) are all Euclidean vectors in \( \mathbb{R}^n \), where \( n \) is the dimension of the underlying space.

To the best of our knowledge, the first paper in MC society that mentions FAP as an information carrying property is [15]. The density function of FAP is derived in closed-form for both pure diffusion and diffusion with a constant drift in 3D spaces. However, this approach is limited in scope when higher dimensional diffusion is considered. Later, the authors in [16] use Green’s function and the method of images to derive the FAP density function for 2D MC systems, where the fluid medium has a constant drift restricted to the longitudinal direction from the transmitter towards the receiver. However, the method of images in [16] cannot be generalized to the setting of arbitrary drift velocity field, which is commonly encountered in fluid environments, because it uses symmetry heavily, but an arbitrary direction of drift will break down the required symmetry. Finally, the capacity of molecular position channels remains completely unknown except some very specific cases, see [16] for capacity of \( M \)-ary modulation scheme.

**C. Our Contributions**

Although most works in MC consider FAT modulation for absorbing receivers, there are at least two reasons why FAP is preferable:

- For each message particle, the FAT information is only one-dimensional, while the FAP could have higher dimensions to carry information. Hence, the capacity of FAP could be larger than FAT per single message particle.
- Practically, “guard intervals” between two consecutive transmissions are required to avoid cross-over effects, as described in Eq. (2). Due to these guard intervals, the total transmission time for FAT-type modulation will increase roughly proportional to the number of MMNs to be transmitted. Consequently, for applications in which the time efficiency plays an important role, the FAP-type modulation is arguably a better solution.

The main contributions of this paper are two-fold. 1) We relax the constraint imposed on the drift direction in previous works. 2) We introduce the semigroup approach to facilitate characterization of the FAP density for planar absorbing receivers in higher dimensional diffusion channels. Our methodology unifies the process toward finding FAP in 2D and 3D with a solid theoretical backup (see Section III for details). Technically, the semigroup approach avoids complicated time integration in finding FAP. We believe that our work opens the possibility toward resolution of the capacity of molecular position channels.

**D. Structure of this Paper**

The remainder of this paper is structured as follows. Section II describes the system model we choose, and some related papers working on FAP. Section III presents the new methodology we proposed to find FAP. Finally, concluding remarks are made in Section IV.

**II. SYSTEM MODEL AND RELATED WORKS**

**A. System Model**

We consider a MC system located in an \( n \)-dimensional Euclidean space, consists of a point \( \text{Tx} \) and a planar absorbing Rx. The distance between \( \text{Tx} \) and \( \text{Rx} \) is \( d \). Notice that we can always arrange the basis of \( \mathbb{R}^n \) so that the last vector in the basis set is parallel to the transmission direction. Without loss of generality, we consider that the transmitter is a point located at the Cartesian coordinate \((0, \ldots, 0, d)\), and the receiver is an infinite large absorbing plane located at \( \{x \in \mathbb{R}^n : x_n = 0\} \). Abstract MC system figures for 2D and 3D spaces are illustrated in Figure 1 and Figure 2 respectively.

The physical channel of our MC model is composed of a diffusive fluid medium with a constant drift. In theoretical MC literature, there are two different viewpoints to model diffusion channels. The macroscopic viewpoint uses diffusion equation (aka heat equation) to capture the evolution of the whole concentration field of message molecules. While in the microscopic viewpoint, individual message molecule is monitored using its own trajectory; namely, the position (as a function of time) of each molecule is a random process. For the equivalence of these two viewpoints, the readers can refer to

[2] Here we use the word “field” to mean a function of space and time.
classical potential theory as in [25], or a good review paper in MC such as [9] or [13].

In the macroscopic viewpoint, the physical channel is modeled by Eq. (3) below. Since the numbers of particles are continuously distributed, the most important quantity in macroscopic MC system analysis is the concentration field \( c(\mathbf{r},t) \) of message molecules at spatial position \( \mathbf{r} \) and time \( t \). By Fick’s law of diffusion [13], the evolution of \( c(\mathbf{r},t) \) can be captured by the diffusion-advection equation:

\[
\frac{\partial c(\mathbf{r},t)}{\partial t} + \mathbf{v}(\mathbf{r},t) \cdot \nabla c(\mathbf{r},t) = D \nabla^2 c(\mathbf{r},t),
\]

where \( \mathbf{r}_0 \) is the point where the diffusion starts, \( \mathbf{v} \) is the velocity field of the fluid medium which is assumed to be incompressible, \( \nabla \) and \( \nabla^2 \) are the gradient and the Laplace operators, respectively, and \( D \) is the diffusion coefficient. The value of \( D \) is determined by the temperature, the fluid viscosity, and the molecule’s Stokes radius, see [9].

On the other hand, in the microscopic viewpoint, a common assumption is that the trajectory of each molecule can be well distinguished. A mainstream model in MC for the trajectory \( X_t \) of a MM is the Itô diffusion process. An Itô diffusion in Euclidean space \( \mathbb{R}^n \) is a stochastic process satisfying a stochastic differential equation of the form

\[
dX_t = b(X_t)dt + \sigma(X_t)dB_t,
\]

where \( B_t \) is an \( n \) dimensional Brownian motion. Throughout this paper, we assume that \( b \) and \( \sigma \) are both constants and can be determined by the fluid and properties of MMs. We further assume that the receiver for our MC system is perfectly absorbing (as described in Section [9]) and has the ability to correctly measure the time and position at first-arrival for each individual molecule [16].

In the following, we denote the initial position of a MM by \( \mathbf{x} \), the final (or received) position by \( \mathbf{y} \), and the FAP density by \( f(\mathbf{y}|\mathbf{x}) \).

B. Related Works

1) 2D FAP density: The authors of [16] solved this problem in 2D partially[3]. In [16], a 2D MC system with a constant drift velocity \( \mathbf{v} \) pointing directly to the receiver is considered. The authors of [16] adopt the method of images to construct Green’s function for an absorbing boundary. The resulting FAP density function can be written as:

\[
f_{Y|X}(\mathbf{y} | \mathbf{x}) = \frac{|\mathbf{v}|d}{2\pi D} \exp \left\{ -\frac{|\mathbf{v}|d}{2D} \right\} \frac{1}{\sqrt{d^2 + (\xi - x_1)^2}}
\]

\[
\times K_1 \left( \frac{|\mathbf{v}| \sqrt{d^2 + (\xi - x_1)^2}}{2D} \right),
\]

where \( D \) is the macroscopic diffusion coefficient, \( d \) is the distance between Tx and Rx, \( \mathbf{x} \) and \( \mathbf{y} \) are position vectors in \( \mathbb{R}^2 \), and \( K_1(\cdot) \) is the modified Bessel function of the first order. Notice that we cannot recover the FAP expression as appeared in [16] Eq. (14)]. Instead, we have provided a self-contained proof in Appendix [A]

2) 3D FAP density: In [15], a 3D MC system with a constant drift velocity \( \mathbf{v} \) pointing to arbitrary direction is considered. The system model is illustrated in Figure 2. The authors of [15] use Dynkin’s formula to link the microscopic properties at first arrival time to the solution of macroscopic diffusion equation. A closed-form FAP density function in 3D is obtained in [15], which has the following form:

\[
f_{Y|X}(\mathbf{y} | \mathbf{x}) = \frac{\lambda}{2\pi} \exp \left\{ -\frac{v_3\lambda}{\sigma^2} \right\} \exp \left\{ \frac{v_2}{\sigma^2} (\xi - x_1) + \frac{v_2}{\sigma^2} (\eta - x_2) \right\} \exp \left\{ -\frac{|v|}{\sigma^2} ||\mathbf{y} - \mathbf{x}|| \right\} \times \frac{1 + \frac{|v|}{\sigma^2} ||\mathbf{y} - \mathbf{x}||}{||\mathbf{y} - \mathbf{x}||^3}
\]

\[
= \frac{\lambda}{2\pi} \exp \left\{ -\frac{v_3\lambda}{\sigma^2} \right\} \exp \left\{ \frac{v_2}{\sigma^2} (\xi - x_1) + \frac{v_2}{\sigma^2} (\eta - x_2) \right\} \exp \left\{ -\frac{|v|}{\sigma^2} ||\mathbf{y} - \mathbf{x}|| \right\} \frac{1 + \frac{|v|}{\sigma^2} ||\mathbf{y} - \mathbf{x}||}{||\mathbf{y} - \mathbf{x}||^3}
\]

where \( \sigma^2 = 2D \) is the microscopic diffusion coefficient, \( d = \lambda \) is the distance between transmitter plane and receiver plane, \( v_3 \) is the component of velocity parallel (or longitudinal) to the information transmission direction, and \( v_1 \) and \( v_2 \) are the components perpendicular (or transverse) to the transmission

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Fig. 1. System Model of 2D First Arrival Position Channels.

Fig. 2. System Model of 3D First Arrival Position Channels.
direction. Here we use the symbol $\| \cdot \|$ to represent the Euclidean norm. Namely,

$$\| y - x \| = \sqrt{(\xi - x_1)^2 + (\eta - x_2)^2 + \lambda^2},$$

(8)

where $x = (x_1, x_2, \lambda)$, $y = (\xi, \eta, 0)$ are position vectors in $\mathbb{R}^3$.

III. GENERATOR OF ITÔ DIFFUSION AND DYNKIN’S FORMULA

By suitably examine macroscopic and microscopic relations, we come up with new ideas to simplify the procedure to finding FAP density. Briefly speaking, after careful thinking, one can realize the FAP density itself does not depend on time, so there must be some redundant calculations during the old methods playing with heat equations, as in [16]. In our new approach, we consider the generator of the diffusion semigroup, rather than the time-dependent heat equation. Through this semigroup approach, the MC channel can be simply regarded as a time-invariant system. This saves lots of grief comparing to other methods bothering with transient effects in heat equation.

Our new approach toward finding the FAP density can be summarized in three key steps:

1. By considering the generator of diffusion semigroup, we can remove the time variable from the very beginning. This is because of the Markov property of diffusion semigroups.
2. The second step is to look up the solution representation forms from PDE literatures for the corresponding elliptic boundary value problems (BVP). Since there are plentiful well known results for solution of elliptic PDEs (even in high dimensional cases, see [26], [27]), we benifit a lot from these existing results in mathematics by transforming our problem into elliptic type.
3. Via correctly interpreting the Dynkin’s formula, we show that the FAP density can be obtained directly by examining

$$f_{Y|X}(y | x) = \left[ \frac{\partial G(y, x)}{\partial n_y} \right],$$

(9)

where $G(y, x)$ is the elliptic Green’s function. Notice that we omit the complicated integration step as appeared in [16] Eq. (17).

The comparisons between the old and new methods are listed in Table I. For the sake of completeness, the old method is briefly reviewed in Appendix B in a self-contained way.

### A. Infinitesimal Generator of Itô Diffusion

An Itô diffusion\(^4\) in Euclidean space $\mathbb{R}^n$ is a stochastic process satisfying a stochastic differential equation of the form

$$dX_t = b(X_t)dt + \sigma(X_t)dB_t,$$

(10)

\(^4\)We merely consider time-homogeneous Itô diffusion throughout this paper. That is, $b(X_t)$ and $\sigma(X_t)$ does not depend on $t$ explicitly.

### TABLE I

| Old Method (with $t$) | New Method (without $t$) |
|-----------------------|--------------------------|
| Step 1 | Find the free space Green's function for parabolic PDE. | Removing time $t$ from the beginning by considering the generator of diffusion. |
| Step 2 | Solve for absorbing Green's function based on image method. | Look up the solution forms for certain types of elliptic BVPs. |
| Step 3 | Calculating FAP density flux and doing time integration. | Interpretate the Dynkin’s formula and obtain the FAP density directly. |

where $B_t$ is an $n$ dimensional Brownian motion. Throughout this paper, we assume that $b$ and $\sigma$ are both constants and can be determined by the fluid and message particle properties.

To each specific Itô diffusion process, we can associate a corresponding operator as follows. Let $\mathcal{D}(A)$ be the domain of the generator and denote

$$\mathbb{E}^x[f(X_t)] := \mathbb{E}[f(X_t)|X_0 = x].$$

(11)

The generator $A$ of a process $X_t$ can be defined as

$$Af(x) = \lim_{t \to 0} \frac{\mathbb{E}^x[f(X_t)] - f(x)}{t} \quad \text{for } f \in \mathcal{D}(A).$$

(12)

For time-homogeneous Itô process, it is a Markov process, so we can also define

$$T_t := \mathbb{E}^x[f(X_t)]$$

(13)

and forming a semigroup $T = (T_t)_{t \geq 0}$. In this language,

$$Af = \lim_{t \to 0} \frac{T_tf - f}{t}$$

(14)

can be regarded as the linear term (omitting all higher order terms) of the semigroup evolution.

Since the FAP problem itself is irrelevant to time variable $t$, our main idea is to remove the time variable $t$ at the beginning, so that the calculation of Green’s functions can be further simplified. The next step is to calculate the generator $A$ explicitly from the Itô diffusion SDE: $dX_t = b(X_t)dt + \sigma(X_t)dB_t$. Supposing $f \in C^2$, by Taylor expansion and Itô’s formula\(^5\), we have

$$d f(X_t) = f' (X_t) dX_t + \frac{1}{2} f'' (X_t) d(X_t)_t$$

(15)

$$= \left[ b(X_t) f' (X_t) + \frac{\sigma^2(X_t)}{2} f'' (X_t) \right] dt + f' (X_t) \sigma (X_t) dB_t.$$ 

The notation $d(X_t)_t$ represents the quadrature variation of random process $X_t$. Comparing to the definition of generator [12], we get:

$$Af(x) = b(x)f'(x) + \frac{\sigma^2(x)}{2} f''(x)$$

(16)

for Itô diffusion.

\(^5\)This is a standard result in stochastic analysis, see [28].
B. Boundary Value Problem for Elliptic PDE

For MC systems which are time-invariant and spatial-homogeneous, we can restrict ourselves to the case that both \( b(x) \) and \( \sigma(x) \) are constants. Consider the PDE boundary value problem (BVP) with unknown function \( u \):

\[
\begin{align*}
  Au = 0 & \quad \text{in } \Omega \\
  u = g & \quad \text{on } \partial\Omega
\end{align*}
\]

(17)

where \( g \) is some prescribed boundary data. For elliptic differential operator \( A \), the solution of (17) under various boundary conditions can be found in standard handbooks of PDE, for instance [26]. Let us discuss a simple example to take a glance of this. Consider \( A = \nabla \cdot \) to be the 3D Laplacian operator in Cartesian coordinate. The solution to

\[
Au = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0
\]

is called the fundamental solution

\[
\mathcal{E}(x, y, z) = \frac{1}{4\pi \sqrt{x^2 + y^2 + z^2}}
\]

(19)

If a half-space domain is considered, and a boundary condition is prescribed:

\[
u = g(x, y) \quad \text{at } z = 0.
\]

(20)

The solution of the BVP is well known and can be look up in standard handbooks of PDE. It has the following form:

\[
u(x, y, z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{zg(\xi, \eta) d\xi d\eta}{(x - \xi)^2 + (y - \eta)^2 + z^2}.
\]

(21)

Eq. (21) is called an integral representation formula in classical PDE language. Rewrite (21) as

\[
u(x, y, z) = \int_{\partial\Omega} \left. \frac{\partial G(\xi, \eta; 0; x, y, z)}{\partial n} \right| g(\xi, \eta) d\xi d\eta.
\]

(22)

We claim that the term

\[
\left. \frac{\partial G(\xi, \eta; 0; x, y, z)}{\partial n} \right|
\]

(23)

is already the FAP density on the receiving plane. In this example, it corresponds to the 3D no-drift case. The above simple example demonstrates the main idea, but we should prove this claim in a more rigorous way, as shown in the following section.

Also note that the right hand side of the first equation in (17) is zero, meaning that there are no particle production and annihilation in the fluid domain.

C. Dynkin’s Formula and First Arrival Position Density

In modern probability theory, the properties of a stopped random process at hitting time is a subtle issue. We will not go through the rigorous details about the stopped process, but just use the Dynkin’s formula to explain the relation between microscopic diffusion and macroscopic phenomena.

Recall that the definition of an infinitesimal generator is

\[
Af(x) = \lim_{t \to 0} \frac{\mathbb{E}^x[f(X_t)] - f(x)}{t}.
\]

(24)

Rewriting the above equation into an integral form, we have

\[
\mathbb{E}^x[f(X_t)] = f(x) + \mathbb{E}^x \left[ \int_0^t Af(X_s) ds \right].
\]

(25)

Note that \( t \) appeared in the above formula is a deterministic variable, not a random variable.

In stochastic analysis, Dynkin’s formula is a theorem giving the expected value of suitably smooth statistic of an Itô diffusion at a stopping time. Let \( f \) be \( C^2 \) with compact support. Let \( \tau \) be a stopping time with \( \mathbb{E}^x[\tau] < +\infty \). Then Dynkin’s formula can be written as

\[
\mathbb{E}^x[f(X_\tau)] = f(x) + \mathbb{E}^x \left[ \int_0^\tau Af(X_s) ds \right].
\]

(26)

The notation \( \mathbb{E}^x[\cdot] \) stands for taking expectation conditioned on \( X_0 = x \).

With these background materials at hand, we can now derive the FAP density from the fundamental solution of elliptic-type BVP in principle. Let \( g \) be a smooth data defined on the boundary (i.e. the receiver plane) of the domain. We can write

\[
\mathbb{E}^x[g(X_\tau)] = \mathbb{E}[g(X_\tau) | X_0 = x] = \int_{\partial\Omega} f_{Y|X}(y | x) g(y) dy
\]

(27)

using the conditional probability density function (PDF) language. Note that \( \tau \) is the hitting time, so \( y \in \partial\Omega \); and \( x \in \Omega \) is the starting point of the diffusion process. By definition, the conditional PDF \( f_{Y|X} \) is the desired FAP density given the starting point of the diffusion is \( x \).

Consider an Itô diffusion \( X_t \) and its corresponding generator \( A \). Suppose we have found a solution \( u(x) \) of the BVP problem

\[
\begin{align*}
  Au = 0 & \quad \text{in } \Omega \\
  u = g & \quad \text{on } \partial\Omega
\end{align*}
\]

(28)

for some prescribed \( g \). Now we plug \( f(x) = u(x) \) into Eq. (26). The last term

\[
\int_0^\tau Au(X_s) ds = 0
\]

(29)

since \( 0 < s < \tau \) and \( \tau \) is the first hitting time, so that \( X_s \) lies in \( \Omega \). On the other hand, the term on the left hand side of Eq. (26) becomes \( \mathbb{E}^x[g(X_\tau)] \) because \( u(x) \) coincides with \( g(x) \) on the boundary. Combining these two facts, we get

\[
\mathbb{E}^x[g(X_\tau)] = u(x) = \int_{\partial\Omega} f_{Y|X}(y | x) g(y) dy
\]

(30)

for any \( x \in \Omega \). For common types of boundary conditions, the solution of Eq. (25) can be written explicitly using representation formulas (see [26]). Generically, for elliptic type problems in domain \( V \) and boundary \( S \), we have

\[
u(x) = \int_V \Phi(y)G(x, y) dV_y + \int_S g(y)H(x, y) dS_y
\]

(31)

where \( \Phi \) represents the source term, \( dV_y \) is the volume element, \( dS_y \) is the surface element, and the term \( H(x, y) \) depends on which type of boundary conditions we are considering.
For the purpose of deriving the FAP density, we can set \( \Phi(y) = 0 \) for all \( y \in V \) and consider the Dirichlet type boundary, i.e.

\[
H(x, y) = -\frac{\partial G}{\partial n_y}(x, y). 
\]

Then formula (31) becomes

\[
u(x) = \int_S \frac{\partial G}{\partial n_y}(x, y) g(y) dS_y. 
\]

Finally, by comparing Eq. (30) and Eq. (33), we reveals an important relation between the FAP density and elliptic Green’s function:

\[
f(y|x)(x) = \left| \frac{\partial G}{\partial n_y}(x, y) \right|. 
\]

IV. CONCLUSIONS

In this paper, we fully resolve the FAP density problem for planar absorbing receivers in MC. Our approach is based on the theory of diffusion semigroups. The comparisons between the existing and our methods are listed in Table I. Through this semigroup approach, we integrate the existing FAP results in 2D and 3D.

Secondly, this is the first paper in MC to clarify in a rigorous way the mathematical link between the macroscopic and microscopic viewpoints for the diffusion mechanism in diffusion-based MC systems. Previous works in MC treat these two viewpoints separately. We hope this clarification could bring new insights into future theoretical MC system analysis.

Finally, we provided a self-contained proof for the formula proposed in [16] for 2D FAP density problem. We also make some improvement via relieving the restriction that the drift direction must point exactly toward the receiver. The calculation details are presented in Appendix A.

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APPENDIX A
CALCULATION OF FAP DENSITY IN 2D SPACE USING SEMIGROUP APPROACH

For two dimensional FAP density calculation, we consider a planar Itô diffusion $X_t$ with its semigroup generator $A$ as

$$A = \sum_{i=1}^{2} v_i \frac{\partial}{\partial x_i} + \sigma^2 \sum_{i=1}^{2} \frac{\partial^2}{\partial x_i^2}. \quad (35)$$

In the above equation, the term $v_i$ stands for the $i$-th component of the drift velocity. Let us denote the Laplacian operator in 2D by $\Delta_2$. Consider the following BVP in Cartesian coordinate:

$$\{ \begin{array}{ll}
A(u) = \sum_{i=1}^{2} v_i \frac{\partial u}{\partial x_i} + \frac{\sigma^2}{2} \Delta_2 u = 0 & \text{in } \Omega \\
u = g & \text{on } \partial \Omega, \end{array} \quad (36)$$

where $u$ is a (dummy) unknown function in PDE language. Set the domain of BVP (36) to be

$$\Omega = \mathbb{R}^2 \cap \{ x_2 > 0 \}, \quad (37)$$

and the boundary to be

$$\partial \Omega = \mathbb{R}^2 \cap \{ x_2 = 0 \}. \quad (38)$$

with notation $x_j$ denoting the $j$-th component of the position vector $x = (x_1, \ldots, x_n)$. For the purpose of compatibility to higher dimensional cases, we arrange the basis of the Cartesian coordinate so that the last component is parallel to the transmission direction.

The BVP (36) is not a common solved form in standard PDE handbooks, for instance [26]. However, we can use a special change of variables to transform (36) into a Helmholtz equation. Before proceeding further, we temporarily set $\sigma^2 = 1$ to avoid cumbersome notations. After obtaining the final result, we will then replace $v_i$ with $\frac{v_i}{\sigma^2}$ to recover the solution for general $\sigma^2$ not necessarily equal to 1.

Suppose $u$ is the solution of BVP (36) with $\sigma^2 = 1$. That is, $u$ satisfies $\sum_{i=1}^{2} v_i \frac{\partial u}{\partial x_i} + \frac{1}{2} \Delta_2 u = 0$ in the domain $\Omega$, and $u$ coincides with the data function $g$ on the boundary $\partial \Omega$. We define a drift factor $\gamma$ to facilitate our calculation, as follows

$$\gamma(x) := \exp \{ \mathbf{v} \cdot \mathbf{x} \} = \exp \{ v_1 x_1 + v_2 x_2 \}, \quad (39)$$

where $\mathbf{v} \cdot \mathbf{x}$ denotes the standard inner product in $\mathbb{R}^2$. By assigning a new function $w(x) = \gamma(x) u(x)$, we plug $u(x) = w(x) / \gamma(x)$ into BVP (36) and get:

$$\frac{1}{\gamma(x)} [\Delta_2 w(x) - (v_1^2 + v_2^2) w(x)] = 0. \quad (40)$$

Next, by letting

$$s = |\mathbf{v}| = \sqrt{v_1^2 + v_2^2}, \quad (41)$$

we can deduce that $w$ satisfies the Helmholtz equation:

$$\Delta_2 w - s^2 w = 0 \quad (s \geq 0). \quad (42)$$

The Helmholtz equation can be regarded as the eigenvalue problem of Laplacian operator; its solution form can be found in standard PDE books [26]. To solve $w$, we consider another BVP described by the Helmholtz equation:

$$\{ \begin{array}{ll}
H(w) = \Delta_2 w - s^2 w = 0 & \text{in } \Omega \\
w = \tilde{g} & \text{on } \partial \Omega, \end{array} \quad (43)$$

Note that the boundary data $\tilde{g}$ after transformation satisfies

$$\tilde{g}(y) = e^{v_1 y_1} g(y) \quad \text{for } y \in \partial \Omega \quad (44)$$

since $y_2 = 0$ on the boundary.

The next step is to look up solution tables for the representation formula of solution of BVP (43). The following equations (47) and (49) are cited from [26].

**Domain:** $-\infty < x_1 < \infty$, $0 \leq x_2 < \infty$. (First boundary value problem.) A half-space is considered. A boundary condition is prescribed:

$$w(x_1, 0) = g(x_1) \quad \text{at } x_2 = 0. \quad (45)$$

**Solution of (43):**

$$w(x_1, x_2) = \int_{-\infty}^{x_1} \int_{-\infty}^{x_2} f(\xi) \left[ \frac{\partial}{\partial \eta} G(x_1, x_2, \xi, \eta) \right]_{\eta=0} d\xi. \quad (46)$$

Green’s function for $\lambda = -s^2 < 0$:

$$G(x_1, x_2, \xi, \eta) = \frac{1}{2\pi} [K_0(s\rho_1) - K_0(s\rho_2)] \quad (47)$$

where

$$\rho_1 = \sqrt{(x_1 - \xi)^2 + (x_2 - \eta)^2}, \quad (48)$$

$$\rho_2 = \sqrt{(x_2 - \xi)^2 + (x_2 + \eta)^2}. \quad (49)$$

Interested readers can refer to [29] for more details about the derivation of this Green’s function.

Now we let $x = (x_1, x_2)$, $y = (\xi, \eta)$. Based on the methodology presented in Section III, we know that

$$w(x) = \int_{\partial \Omega} \left[ \frac{\partial G(x, y)}{\partial n_y} \right] \tilde{g}(y) dy. \quad (50)$$

Here, the notation $|\frac{\partial G(x, y)}{\partial n_y}|$ is the partial derivative of $G$ with respect to the direction normal to the boundary $\partial \Omega$. Using the fact that $K_0'(x) = -K_1(x)$, we calculate

$$\left| \frac{\partial G}{\partial \eta} \right| = \frac{\partial G}{\partial \rho_1} \frac{\rho_1}{\rho_1} + \frac{\partial G}{\partial \rho_2} \frac{\rho_2}{\rho_2} \bigg|_{\eta=0} = -\frac{s}{2\pi} K_1 \left( \sqrt{(x_1 - \xi)^2 + x_2^2} \right) \frac{-x_2}{\sqrt{(x_1 - \xi)^2 + x_2^2}}$$

$$+ \frac{s}{2\pi} K_1 \left( \sqrt{(x_1 - \xi)^2 + x_2^2} \right) \frac{x_2}{\sqrt{(x_1 - \xi)^2 + x_2^2}}$$

$$= \left| \frac{\rho_1}{\rho_2} \right| \frac{K_1 \left( \sqrt{(x_1 - \xi)^2 + x_2^2} \right)}{\pi \sqrt{(x_1 - \xi)^2 + x_2^2}}. \quad (51)$$
To obtain a representation formula for the solution $u$ of the original BVP (50), we substitute $w(x) = \gamma(x)u(x)$ into (50), yielding

$$u(x) = \frac{w(x)}{\gamma(x)} = \exp(-v \cdot x) \int_{\partial \Omega} \left| \frac{\partial G(x, y)}{\partial n_y} \right| g(y) dy = \int_{\partial \Omega} \exp \left\{ v_1 y_1 - v_1 x_1 - v_2 x_2 \right\} \left[ \frac{\partial G}{\partial n_1} \frac{\partial G}{\partial \eta_1} + \frac{\partial G}{\partial n_2} \frac{\partial G}{\partial \eta_2} \right]_{\eta=0} g(y_1) dy_1 = \int_{\partial \Omega} K_v(x, \xi) g(\xi) d\xi,$$

where $K_v(x, \xi)$ is some integral kernel which we want to determine. Note that in the second equality of (52), we have used the relation $g(y_1) = e^{v_1 y_1} g(y_1)$.

Now let $x_2 = d > 0$ to be the transmission distance between Tx and Rx. By examining equation (52), we obtain an exact formula for the Markov probability kernel $K_v(x, \xi)$:

$$K_v(x, \xi) = \exp \left\{ v_1 \xi - v_1 x_1 - v_2 d \right\} \left[ \frac{\partial G}{\partial n_1} \frac{\partial G}{\partial \eta_1} + \frac{\partial G}{\partial n_2} \frac{\partial G}{\partial \eta_2} \right]_{\eta=0} \frac{|v| d \exp(-v_2 d) \exp(-v_1 (x_1 - \xi))}{K_1 \left( \frac{|v|}{\sigma^2} \sqrt{(x_1 - \xi)^2 + d^2} \right) \sqrt{(x_1 - \xi)^2 + d^2}}$$

(53)

To tackle with the general case $\sigma^2 \neq 1$, we can just replace $v_1$ with $\frac{v_1}{\sigma^2}$, yielding

$$f_{Y \mid X}(y \mid x) = \frac{|v| d}{\sigma^2 \pi} \exp \left\{ -\frac{-v_2 d}{\sigma^2} \right\} \exp \left\{ -\frac{-v_1 (x_1 - \xi)}{\sigma^2} \right\} \frac{K_1 \left( \frac{|v|}{\sigma^2} \sqrt{(x_1 - \xi)^2 + d^2} \right)}{\sqrt{(x_1 - \xi)^2 + d^2}},$$

(54)

where $x = (x_1, d)$, $y = (\xi, 0)$, and $d$ is the distance between the transmitter and the receiver plane. Equation (54) is the desired conditional density function (allowing arbitrary drift directions) for 2D FAP problem.

In order to make comparison to the more restrictive result in [16], we can set $v_1 = 0$ in equation (54), yielding

$$f_{Y \mid X}(y \mid x) = \frac{|v| d}{\sigma^2 \pi} \exp \left\{ -\frac{-v_2 d}{\sigma^2} \right\} \frac{K_1 \left( \frac{|v|}{\sigma^2} \sqrt{(x_1 - \xi)^2 + d^2} \right)}{\sqrt{(x_1 - \xi)^2 + d^2}}$$

(55)

where we use the relation $\sigma^2 = 2D$.

APPENDIX B

THE OLD METHOD: SEPARATION OF VARIABLES AND METHOD OF IMAGE

For the sake of completeness, we briefly review the original approach to finding FAP density function as proposed in [16].

A. Finding the Green’s Function for Free Space

For a 2-dimensional diffusion channel, with a constant drift velocity $v$ from the transmitter to the receiver along the $x$-axis, equation (4) can be rewritten as

$$\frac{\partial c(x, y, t)}{\partial t} + v \frac{\partial c(x, y, t)}{\partial x} = D \left( \frac{\partial^2 c(x, y, t)}{\partial x^2} + \frac{\partial^2 c(x, y, t)}{\partial y^2} \right)$$

(56)

where, $c(x, y, 0) = \delta (x - x_0) \delta (y - y_0)$ is the 2-dimensional Dirac delta function, and $c(x, y, t) = 0$, for $x, y \in \partial \Omega$.

Using separation of variables, the concentration field $c(x, y, t)$ can be written as $c(x, y, t) = c_1(t) c_2(y, t)$. By plugging back into equation (56), we can get two separated equations

$$\frac{\partial c_1}{\partial t} + v \frac{\partial c_1}{\partial x} = D \frac{\partial^2 c_1}{\partial x^2} = 0,$$

$$\frac{\partial c_2}{\partial t} + v \frac{\partial c_2}{\partial y} = D \frac{\partial^2 c_2}{\partial y^2} = 0.$$

(57, 58)

The fundamental solutions of these two sub-equations are

$$c_1(t) = \frac{1}{\sqrt{4 \pi D t}} \exp \left( -\frac{(x - x_0 - vt)^2}{4Dt} \right)$$

(59)

and

$$c_2(y, t) = \frac{1}{\sqrt{4 \pi D t}} \exp \left( -\frac{(y - y_0)^2}{4Dt} \right).$$

(60)

Hence the Green’s function of (56) can be written as the product of the above two concentrations:

$$G(x, y, x_0, y_0, t) = \frac{1}{4 \pi D t} \exp \left( -\frac{(x - x_0 - vt)^2 - (y - y_0)^2}{4Dt} \right).$$

(61)

B. Finding the Green’s Function for Absorbing Boundary

Until now, we have not yet taken the boundary conditions into account. From the original physical problem, we know that the receiver is a plane (or “line” in 2-d). Since the receiver is assume to be perfectly absorbing, we set the concentration field to be zero on the boundary.

There is one well-known technique (originated in classical electrodynamics) that works well for boundaries with flat surfaces, called the method of image, see [30]. Since we only care about the concentration in the domain, we can effectively put an image source of negative mass at the reflection point of the original releasing point to replace the boundary effect. Namely, we write

$$G_{abs}(x, y, x_0, y_0, t) = G(x, y, x_0, y_0, t) - a(x_0)G(x, y, -x_0, y_0, t)$$

(62)
and then solve for \( a(x_0) \). The subscript \( \text{abs} \) stands for “absorbing”. The absorbing boundary condition gives

\[
a(x_0) = \frac{G(0, y, x_0, y_0, t)}{G(0, y, -x_0, y_0, t)} = \exp \left( -\frac{x_0 v}{D} \right). \tag{63}
\]

We can now write down the Green’s function for absorbing boundary as

\[
G_{\text{abs}}(x, y, x_0, y_0, t) = \frac{1}{4\pi Dt} \left[ \exp \left( -\frac{(x - x_0 - vt)^2 + (y - y_0)^2}{4Dt} \right) \right] - \exp \left( -\frac{x_0 v}{D} \right) \]. \tag{64}
\]

C. From Green’s function to First Arrival Position Density

Consider the diffusive flux \( J(0, y, t) \) at \( x = 0 \), which has a unit of particle density per unit length and unit time. By Fick’s law, we know that

\[
J(0, y, t) = -D \frac{\partial G_{\text{abs}}(x, y, x_0, y_0, t)}{\partial x} . \tag{65}
\]

Using the absorbing Green’s function formula obtained in (64), we can calculate the flux explicitly, resulting

\[
J(0, y, t) = -\frac{x_0}{4\pi Dt^2} \exp \left( -\frac{(x_0 + vt)^2 + (y - y_0)^2}{4Dt} \right). \tag{66}
\]

Note that the original formula in [16] has some calculation error, so we correct the formula herein.

Our goal is to find the first arrival position density. Let \( X = (x_0, y_0) \) denote the point of release of the information molecule and \( Y = (x, y) \) its arrival position at the receiver boundary. The conditional PDF of \( Y \) at a receiver located at \( x = 0 \) is given as

\[
f_{Y \mid X}(0, y \mid x_0, y_0) = \int_0^\infty J(0, y, t)dt. \tag{67}
\]

Using the diffusion flux we just obtained, we can write

\[
f_{Y \mid X}(0, y \mid x_0, y_0) = -\int_0^\infty \frac{x_0}{4\pi Dt^2} \exp \left( -\frac{(x_0 + vt)^2 + (y - y_0)^2}{4Dt} \right) dt. \tag{68}
\]

To do this integration explicitly, we rearrange the terms to get

\[
f_{Y \mid X}(0, y \mid x_0, y_0) = -\frac{x_0}{4\pi D} \exp \left( -\frac{x_0 v}{2D} \right) \times \int_0^\infty \frac{1}{t^2} \exp \left( -\frac{x_0^2 + (y - y_0)^2}{4Dt} - \frac{v^2 t}{4D} \right) dt. \tag{69}
\]

If \( K_s(z) \) is the modified Bessel function of the second kind, then for positive constants \( a \) and \( b \), we have the relation

\[
\int_0^\infty t^{s-1} \exp \left( -\frac{a}{t} + bt \right) dt = 2 \left( \frac{b}{a} \right)^{s/2} K_s(2\sqrt{ab}), \tag{70}
\]

where \( s \) and \( z \) are real and complex numbers, respectively. Using (69) and (70) and substituting \( x_0 = d \), we finally get

\[
f(y \mid y_0) = f_{Y \mid X}(0, y \mid d, y_0)
\]

\[
= |v|d \exp \left( -\frac{dv}{2D} \right) \frac{1}{\sqrt{D^2 + (y - y_0)^2}} K_1 \left( \frac{|v| \sqrt{D^2 + (y - y_0)^2}}{2D} \right). \tag{71}
\]

Scanning through formula (71), it is worth noting that the conditional FAP density depends only on \( y - y_0 \), hence the FAP channel is an additive (time-invariant) channel.