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Transposition Errors in Diffusion-Based Mobile Molecular Communication

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***Abstract*—In this work, we investigate diffusion-based molecular communication between two mobile nano-machines. We derive a closed-form expression for the first hitting time distribution, by characterizing the motion of the information particles and the nano-machines via Brownian motion. We validate the derived expression through a particle-based simulation. For the information transfer we consider single particles of different types, where transposition errors are the dominant source of errors. We derive an analytical expression for the expected bit error probability and evaluate the error performance for the static and the mobile case by means of computer simulations.**

***Index Terms*—Brownian motion, double random walk channel, first hitting time, mobile molecular communication, transposition error.**

I. Introduction

Molecular communication (MolCom) broadly defines the transmission of information using chemical signals [1]. The information can be encoded in the number of particles, the release time of particles and the type of particles. Diffusion-based MolCom is a promising approach due to its ultra-high energy efficiency [2] and biocompatibility. Since the potential applications of MolCom are in the area of nano-medicine or nano-sensing (e.g., communicating nanorobots for targeted drug delivery [1]), it is likely that the communication takes place between mobile nano-machines.

Mobile MolCom has been considered in [3]–[10]. A clock synchronization scheme between a static and a mobile nanomachine is proposed in [3]. A protocol for mitigating intersymbol interference for diffusion-based mobile MolCom is presented in [4]. Similarly, the work in [5] investigates different coding strategies for mitigating transposition errors for flow-induced diffusion mobile MolCom. In the works [3]–[5] the mobility of the nano-machines is modeled through a time-varying distance (e.g., distance increases with equal difference [3]). Mobile bacteria networks are proposed in [6], applying an i.i.d. mobility model. That is, in each time-slot a network node chooses its new position independently and identically distributed over the entire network. Mobile ad-hoc nano-networks are considered in [7] and [8], where the mobile nano-machines freely diffuse in a three-dimensional (3D) environment via Brownian motion. In [7] the information transfer is accomplished through neurospike communication after collision and adhesion of the nodes and in [8] it based on Förster resonance energy transfer if the nodes are in close proximity of each other. A mathematical model of non-diffusive mobile MolCom networks is presented in [9], describing the two-dimensional mobility of the nano-machines through the Langevin equations. Recently, a systematic approach for modeling time-variant channels for diffusive mobile MolCom systems is proposed in [10]. Similar to [7] and [8], the mobility of the nano-machines is characterized by a 3D Brownian motion model. But in contrast to [7]–[9], the information transfer is accomplished through freely diffusing particles. The channel impulse response of the time-variant channel is derived by modifying the diffusion coefficient of the information particles.

In this letter, we derive a closed-form expression for the first hitting time distribution for diffusion-based mobile MolCom. Similar to [10], we characterize the movement of the nanomachines by Brownian motion. However, unlike [10] we incorporate the variation of the transmitter position in the derivation of the first hitting time distribution. We consider MolCom systems that use single particles of different types to transfer information. In such systems, transposition errors are the dominant source of errors and, thus, fundamentally limit the performance [11]. We derive an analytical expression for the expected bit error probability and evaluate the error performance for the static and mobile case by means of computer simulations.

II. System Model

We consider a semi-infinite one-dimensional (1D) fluid environment, whereby the length of propagation is large compared to width dimensions. We assume constant temperature and viscosity. A point source transmitter nano-machine (TX) and a point receiver nano-machine (RX) are placed in a row at a certain distance. We assume that the TX sends K information bits $\mathbf{b} = [b_0, \ldots, b_{K-1}]^{\mathrm{T}}$ to the RX, where $b_k \in \{0, 1\}$ denotes the transmitted bit in the kth bit interval. As modulation scheme, we adopt binary molecule shift keying [1]. At the beginning of an interval, the TX releases a single type-A or type-B particle to send bit 0 or bit 1, respectively. Each released particle propagates independently via Brownian motion. The RX detects the type of the particle and removes it from the environment, referring to a fully absorbing receiver [12]. The transmitted bits are estimated based on the particle type and their order of arrival [11]. We assume no background noise, i.e. no other particles than type-A and type-B are in the environment. Due to the stochastic nature of the channel, the particles arrive at the RX at random time. The arrival time of a particle released at time $T_{x_k} = kT$, i.e. at the beginning of the kth bit interval with duration T, is given by $T_{y_k} = T_{x_k} + T_n$. The random propagation time until the first

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arrival is denoted by T_n, which is hereafter referred to as first hitting time. In the next section, we discuss the distribution of the first hitting time for non moving as well as moving TX and RX.

III. First Hitting Time Distribution

In this section, we first revisit the first hitting time distribution for fixed TX and RX and then we derive a closed-form expression for the first hitting time distribution, considering a moving TX and RX.

A. Fixed Transmitter and Receiver

Assuming a fixed TX and RX, the first hitting time for 1D diffusion-based channels with no flows follows a Lévy distribution. Its probability density function (PDF) is given by [13]

$$f_{T_n}(t_n) = \frac{R_0}{\sqrt{4\pi D_\mathrm{p} t_n^3}} \exp\left(-\frac{R_0^2}{4D_\mathrm{p} t_n}\right), \quad t_n > 0, \qquad (1)$$

where R_0 denotes the Euclidean distance between TX and RX and D_p is the diffusion coefficient of the information particles.

B. Mobile Transmitter and Receiver

We now assume that TX and RX diffuse with diffusion coefficients D_tx and D_rx, respectively, and that the movement does not disrupt the diffusion process of the information particles. We model the movement of TX and RX as 1D Gaussian random walk (cf. motion of the information particles [1]). We assume that TX and RX move independently of each other and that they cannot pass through each other. Possible collisions between TX and RX are considered by exploiting the equivalence between interacting and noninteracting particles presented in [14]. In particular, it is shown in [14] that except for the particle labeling the space-time trajectories of two interacting particles are equivalent to the space-time trajectories of the non-interacting particles. In other words, the distance between TX and RX after collision is equivalent to the distance if they walk through each other. In the following, we first derive a closed-form expression for the first hitting time distribution taking into account a moving TX and RX and then we evaluate the derived expression for different parameters and verify it through a particle-based simulation.

1) Derivation: First we consider the case of a moving RX and a static TX. To obtain the first hitting time distribution we apply the concept of relative diffusion from [15]. It states that the absorption of information particles by a moving RX can be accurately described by assuming a static RX and particles diffusing with an effective diffusion coefficient defined by the summation of the individual diffusion coefficients. Thus, the first hitting time distribution for a mobile RX and a fixed TX is given by (1), substituting D_p by $D_\mathrm{p,eff} = D_\mathrm{p} + D_\mathrm{rx}$.

Next we consider the relative movement of TX and RX and determine the distribution of the Euclidean distance between them at certain intervals. We define the initial position of TX and RX at time $t = 0$ by the x-coordinates $x_{0,\mathrm{tx}}$ and $x_{0,\mathrm{rx}}$, respectively. Hence, the initial Euclidean distance is given by $R_0 = \sqrt{(x_{0,\mathrm{tx}} - x_{0,\mathrm{rx}})^2}$ (cf. (1)). The motion of TX and RX is described by a sequence of x-coordinates $x_{k,\mathrm{tx}}$ and $x_{k,\mathrm{rx}}$, each coordinate representing the position at the time $t = kT$ (kth interval) [1]. Hence, the Euclidean distance between TX and RX at the time $t = kT$ is given by

$$R_k = \sqrt{(x_{k,\mathrm{tx}} - x_{k,\mathrm{rx}})^2} = \sqrt{d_k^2}, \qquad (2)$$

with $x_{k,u} = x_{0,u} + \sum_{i=1}^{k} \Delta x_u,\ u \in \{\mathrm{tx}, \mathrm{rx}\}$, and $d_k = (x_{k,\mathrm{tx}} - x_{k,\mathrm{rx}})$. The random displacement of TX and RX during the interval duration T is denoted by Δx_u and follows a Gaussian distribution with zero mean and variance $\sigma_u^2 = 2D_u T$ [1]. Thus, the actual position $x_{k,u}$ and the distance d_k follow a Gaussian distribution

$$x_{k,u} \sim \mathcal{N}(x_{0,u}, k\sigma_u^2) \qquad (3)$$

$$d_k \sim \mathcal{N}(d_0, \sigma_k^2), \qquad (4)$$

with $d_0 = x_{0,\mathrm{tx}} - x_{0,\mathrm{rx}}$ and $\sigma_k^2 = k(\sigma_\mathrm{tx}^2 + \sigma_\mathrm{rx}^2)$. To determine the distribution of the Euclidean distance R_k the following definitions are helpful.

Definition 1. *If X is a Gaussian random variable with mean μ and variance σ^2, the random variable $Y = \sqrt{X^2/\sigma^2}$ follows a noncentral chi distribution with one degree of freedom. The PDF is given by*

$$f_Y(y) = e^{-\frac{y^2+\lambda^2}{2}} \sqrt{\lambda y}\, I_{-1/2}(\lambda y),$$

with the noncentrality parameter $\lambda = \sqrt{\mu^2/\sigma^2}$ and the modified Bessel function of the first kind $I_{-1/2}(y)$.

Property 1. *If X has the PDF $f_X(x)$ and $Y = aX$, then Y has the PDF $f_Y(y) = 1/|a| f_X(y/a)$.*

With Definition 1 and Property 1, we can obtain the PDF of the Euclidean distance R_k as follows.

Theorem 1. *Since the distance d_k follows a Gaussian distribution, the Euclidean distance $R_k = \sqrt{\sigma_k^2}\sqrt{d_k^2/\sigma_k^2}$ follows a scaled noncentral chi distribution. The PDF is given by*

$$f_{R_k}(r_k) = \frac{1}{\sqrt{\sigma_k^2}} \left[e^{-\frac{\left(\frac{r_k}{\sqrt{\sigma_k^2}}\right)^2 + \lambda^2}{2}} \sqrt{\lambda \frac{r_k}{\sqrt{\sigma_k^2}}}\, I_{-1/2}\left(\lambda \frac{r_k}{\sqrt{\sigma_k^2}}\right) \right], \qquad (5)$$

with $\lambda = \sqrt{d_0^2/\sigma_k^2}$.

Proof. Multiplying the numerator and denominator of the Euclidean distance R_k defined in (2) with $\sqrt{\sigma_k^2}$ results in

$$R_k = \sqrt{\sigma_k^2}\sqrt{\frac{d_k^2}{\sigma_k^2}} = \sqrt{\sigma_k^2}\tilde{R}_k.$$

with $\tilde{R}_k = \sqrt{d_k^2/\sigma_k^2}$. Using Definition 1, the random variable $\tilde{R}_k$ follows a noncentral chi distribution with the PDF

$$f_{\tilde{R}_k}(\tilde{r}_k) = e^{-\frac{\tilde{r}_k^2+\lambda^2}{2}} \sqrt{\lambda \tilde{r}_k}\, I_{-1/2}\left(\lambda \tilde{r}_k\right),$$

and the noncentrality parameter $\lambda = \sqrt{d_0^2/\sigma_k^2}$. The PDF of the Euclidean distance $R_k = \sqrt{\sigma_k^2}\tilde{R}_k$ can be found using Property 1

$$f_{R_k}(r_k) = \frac{1}{\sqrt{\sigma_k^2}} f_{\tilde{R}_k}\left(\frac{r_k}{\sqrt{\sigma_k^2}}\right).$$

□

We are now interested in the distribution of the first hitting time for a particle released at time $t = T_{x_k} = kT$, taking into account the mobility of TX and RX. This is accomplished by considering the relative motion of the RX and the particles as well as the relative movement of TX and RX. Formally, we derive the PDF of the first hitting time for the mobile case from the first hitting time PDF for the static case defined in (1), with D_p substituted by $D_\text{p,eff}$, and by considering the distance between TX and RX as random variable distributed according to (5). The resulting PDF is parametrized by the discrete time step k and can be calculated for $t_n > 0$ as

$$\begin{aligned} f_{T_n}(t_n;k) =& \int\limits_{r_k=0}^{\infty} f_{T_n|R_k}(t_n|r_k) f_{R_k}(r_k)\mathrm{d}r_k, \\ =& \frac{\sqrt{kTD_\text{tot}D_\text{p,eff}}}{\pi\sqrt{t_n}(kTD_\text{tot} + D_\text{p,eff}t_n)} e^{\frac{-R_0^2}{4kTD_\text{tot}}} \\ &+ f_{T_n}(t_n + kTD_\text{tot}/D_\text{p,eff}) \\ &\times \text{erf}\left(\frac{R_0}{2}\sqrt{\frac{D_\text{p,eff}t_n}{kTD_\text{tot}(kTD_\text{tot} + D_\text{p,eff}t_n)}}\right), \end{aligned} \tag{6}$$

with $D_\text{tot} = D_\text{tx} + D_\text{rx}$ and $f_{T_n}(t_n)$ corresponds to the first hitting time PDF for fixed TX and RX defined in (1). The error function $\text{erf}(x)$ is defined by $\text{erf}(x) = 2/\sqrt{\pi}\int_0^x e^{-t^2}\mathrm{d}t$. Note that when $D_\text{tx} = D_\text{rx} = 0\,\text{m}^2/\text{s}$, i.e. fixed TX and RX, the PDF in (6) turns into the PDF of a Lévy distribution as given in (1).

2) Evaluation: We adopt the parameters[1] proposed in [10] for evaluating the PDF of the first hitting time defined in (6): $R_0 = 1\,\mu\text{m}$, $D_\text{p} = 5\times10^{-10}\,\text{m}^2/\text{s}$, $T = 0.3\,\text{ms}$ and $K = 10$. Figs. 1 and 2 show the impact of different TX and RX mobility as well as the influence of transmitting at different intervals k, on the first hitting time. If the mobility of TX and RX and the interval number k increases, we observe a non-zero probability for a small first hitting time. This is because, in this case the variation of the distance between TX and RX becomes larger (cf. (4)), which results in a non-zero probability that they are in close proximity. It is important to note that for low mobility and a small interval number the second term on the right hand side of (6) mainly determines the PDF, whereas the first term (6) is dominant in case of high mobility and a large interval number. The transition between these two regions can be observed in Fig. 2 for $D_\text{rx} = 5\times10^{-11}\,\text{m}^2/\text{s}$. We verified the formulation of the first hitting time distribution in (6), through simulating the movement of TX and RX as well as the motion of the information particles using Brownian motion [1] and determining the relative frequency of the first particle arrivals. From Figs. 1 and 2 we observe a good match between analytical and simulation results.

Fig. 3 shows the probability of a particle arrival during the interval duration $T = 0.3\,\text{ms}$, when the particle is released at different intervals k, i.e. $F_{T_n}(T;k) = \int_0^T f_{T_n}(t_n;k)\mathrm{d}t_n$. We observe that the arrival probability decreases as the interval number k increases. Similarly, for a certain interval number k, the arrival probability decreases as the mobility increases. This is because, the probability for a large distance between TX and RX becomes higher if the interval number k and/or the mobility increases (cf. (4)), which results in a higher propagation time. Ultimately, the arrival probability during the interval T becomes zero for $k\to\infty$ and/or $D_\text{tx}, D_\text{rx}\to\infty$.

[1] We assume a similar diffusion coefficient for type-A and type-B particles, i.e. $D_\text{p} = D_\text{p,A} = D_\text{p,B}$.

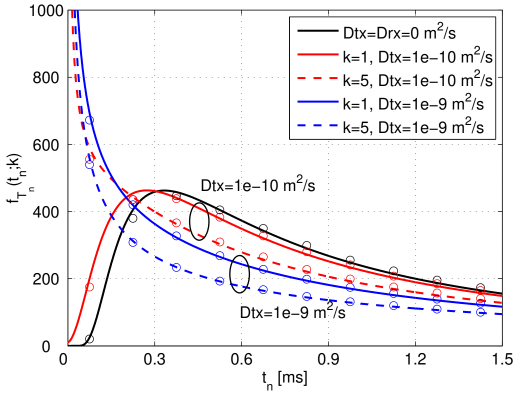

Fig. 1. Evaluation of the PDF $f_{T_n}(t_n;k)$ for different values of D_tx and k, with $D_\text{rx} = 0.5\times10^{-12}\,\text{m}^2/\text{s}$. The results of the particle-based simulation are indicated by $\circ$.

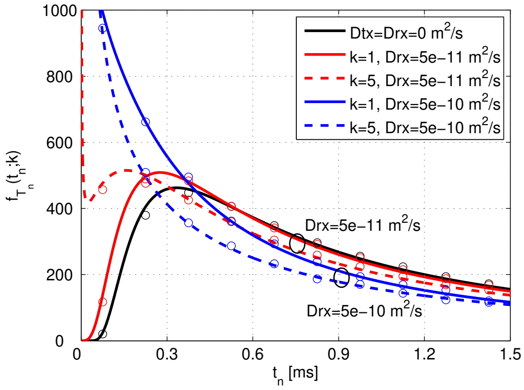

Fig. 2. Evaluation of the PDF $f_{T_n}(t_n;k)$ for different values of D_rx and k, with $D_\text{tx} = 1\times10^{-12}\,\text{m}^2/\text{s}$. The results of the particle-based simulation are indicated by $\circ$.

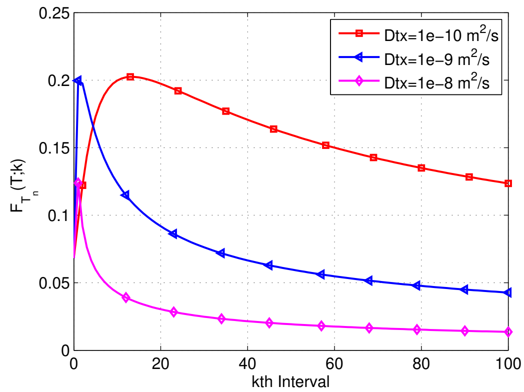

Fig. 3. Probability of a particle arrival during the interval duration $T = 0.3\,\text{ms}$, when the particle is released at the time $t = kT$, i.e. $F_{T_n}(T;k) = \int_0^T f_{T_n}(t_n;k)\mathrm{d}t_n$.

IV. Impact of Mobility on Transposition Errors

In this section, we investigate the impact of mobility on the performance of MolCom systems that use single particles for the information transfer (cf. Section II). Due to the random arrival time of the particles, they may arrive out of order and, thus, particle transpositions occur. Since we assume no background noise, transposition errors are the dominant source of errors and fundamentally limit the performance of such systems [11]. The expected bit error probability for a transmission of K bits can be calculated as [16]

$$P_b = \sum_{\pi \in \mathcal{P}} P_{\text{perm}}(\pi) P_b(\pi), \tag{7}$$

where $\mathcal{P}$ represent the set of all possible permutations on K released particles. The probability that a certain permutation $\pi \in \mathcal{P}$ arrives at the receiver is given by

$$P_{\text{perm}}(\pi) = \int_0^{\infty} \int_{-\infty}^{t_{y_{\pi(K-1)}}} \cdots \int_{-\infty}^{t_{y_{\pi(1)}}} \prod_{i=1}^{K} f_{T_n}(t_{y_{\pi(K-i)}} - T_{x_{\pi(K-i)}}; i) \mathrm{d}t_{y_{\pi(0)}} \cdots \mathrm{d}t_{y_{\pi(K-1)}}, \tag{8}$$

where $f_{T_n}(t_n; k)$ denotes the PDF of the first hitting time defined in (6). The release time of the kth particle is denoted by $T_{x_k} = kT$ (cf. Section II) and $\pi(i)$ denotes the ith element of the permutation π. The expected bit error probability for a certain permutation can be obtained as follows

$$P_b(\pi) = \frac{\text{disp}(\pi)}{2K}, \quad \pi \in \mathcal{P}, \tag{9}$$

where we denote the number of displacements of a permutation π by $\text{disp}(\pi) = \sum_{i=1}^{K} \lceil |\pi(i) - i| / K \rceil$ and $\lceil x \rceil$ corresponds to the mapping to the smallest following integer number.
Fig. 4 shows the bit error ratio (BER) versus the bit interval duration T for different mobility levels of TX and RX[2]. For the BER simulations, we used the parameters from Section III-2). As expected, for the static case the BER degrades if the interval duration T increases. This is also the case if TX and RX are moving, but only up to a certain interval duration T. Then, we observe an error floor, that becomes lower when the mobility decreases.

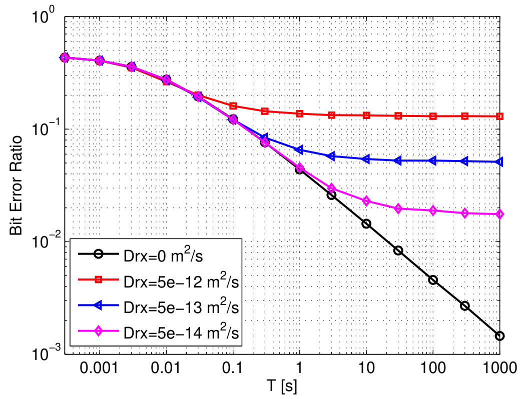

Fig. 4. Bit error ratio versus the bit interval duration T with $D_{\text{tx}} = D_{\text{rx}}$.

V. Conclusions

We derived a closed-form expression for the first hitting time distribution for diffusion-based mobile MolCom. For this, we modeled the movement of the nano-machines by a Gaussian random walk and considered the relative motion of the RX and the particles as well as the relative movement of TX and RX. Moreover, we investigated the impact of mobility on the error performance of MolCom systems that employ single particles of different types to transfer information. In such systems, transposition errors are the dominant source of errors. We derived an analytical expression for the expected bit error probability and computer simulation showed that due to mobility the performance degrades and an error floor appears.

[2]Please note that the calculation of the expected bit error probability in (7) is only possible for small values of K, since $\mathcal{P}$ has $K!$ elements. Thus, we did not include analytical results in Fig. 4. However, a good match between analytical and simulation results was shown in [16] for small values of K and static TX and RX.

References

[1] N. Farsad, H. B. Yilmaz, A. W. Eckford, C. Chae, and W. Guo, "A comprehensive survey of recent advancements in molecular communication," *IEEE Commun. Surveys Tuts.*, vol. 18, no. 3, pp. 1887–1919, thirdquarter 2016.

[2] C. Rose and I. Mian, "A fundamental framework for molecular communication channels: Timing and payload," in *Proc. IEEE Int. Conf. Communications*, June 2015, pp. 1043–1048.

[3] Z. Luo, L. Lin, and M. Ma, "Offset estimation for clock synchronization in mobile molecular communication system," in *Proc. IEEE Wireless Communications and Networking Conference*, April 2016, pp. 1–6.

[4] Y. Sun, M. Ito, and K. Sezaki, "Adaptive code width protocol for mitigating intersymbol interference in diffusion-based molecular communication with mobile nodes," in *Proc. IEEE Int. Conf. e-Health Networking, Applications and Services*, Sept. 2016, pp. 1–6.

[5] S. Qiu, T. Asyhari, and W. Guo, "Mobile molecular communications: Positional distance codes," in *Proc. IEEE Workshop Signal Processing Advances Wireless Communications*, July 2016, pp. 1–6.

[6] W. K. Hsu, M. R. Bell, and X. Lin, "Carrier allocation in mobile bacteria networks," in *Proc. Asilomar Conference on Signals, Systems and Computers*, Nov. 2015, pp. 59–63.

[7] A. Guney, B. Atakan, and O. B. Akan, "Mobile ad hoc nanonetworks with collision-based molecular communication," *IEEE Trans. Mobile Comput.*, vol. 11, no. 3, pp. 353–366, Mar. 2012.

[8] M. Kuscu and O. B. Akan, "A communication theoretical analysis of FRET-based mobile ad hoc molecular nanonetworks," *IEEE Trans. Nanobiosci.*, vol. 13, no. 3, pp. 255–266, Sept. 2014.

[9] S. Iwasaki, J. Yang, and T. Nakano, "A mathematical model of non-diffusion-based mobile molecular communication networks," *IEEE Commun. Lett.*, vol. PP, no. 99, pp. 1–1, 2017.

[10] A. Ahmadzadeh, V. Jamali, A. Noel, and R. Schober, "Diffusive mobile molecular communications over time-variant channels," *IEEE Commun. Lett.*, vol. PP, no. 99, pp. 1–1, 2017.

[11] P. J. Shih, C. H. Lee, P. C. Yeh, and K. C. Chen, "Channel codes for reliability enhancement in molecular communication," *IEEE J. Sel. Areas Commun.*, vol. 31, no. 12, pp. 857–867, Dec. 2013.

[12] H. B. Yilmaz, A. C. Heren, T. Tugcu, and C. B. Chae, "Three-dimensional channel characteristics for molecular communications with an absorbing receiver," *IEEE Commun. Lett.*, vol. 18, no. 6, pp. 929–932, June 2014.

[13] N. Farsad, W. Guo, C. B. Chae, and A. Eckford, "Stable distributions as noise models for molecular communication," in *Proc. IEEE Global Telecommunications Conference*, Dec. 2015, pp. 1–6.

[14] T. E. Harris, "Diffusion with "collisions" between particles," *Journal of Applied Probability*, vol. 2, pp. 323–338, 1965.

[15] H. Kim and K. J. Shin, "Exact solution of the reversible diffusion-influenced reaction for an isolated pair in three dimensions," *Phys. Rev. Lett.*, vol. 82, pp. 1578–1581, Feb. 1999.

[16] W. Haselmayr, S. M. H. Aejaz, A. S. Taufiq Asyhari, and W. Guo, "On the impact of transposition errors in diffusion-based channels," 2017, submitted for publication [Online]. Available: https://128.84.21.199/abs/1701.02971.