Abstract—We consider a multi-link diffusion-based molecular communication (MC) system where multiple spatially distributed transmitter (TX)-receiver (RX) pairs establish point-to-point communication links employing the same type of signaling molecules. To exploit the full potential of such a system, an in-depth understanding of the interplay between the spatial link density and inter-link interference (ILI) and its impact on system performance is needed. In this paper, we consider a three-dimensional unbounded domain with multiple spatially distributed point-to-point non-cooperative transmission links, where both the TXs and RXs are positioned on a regular fixed grid. For this setup, we first derive an analytical expression for the channel impulse responses (CIRs) between the TXs and RXs in the system. Then, we derive the maximum likelihood (ML) detector for the RXs and show that it reduces to a threshold-based detector. Moreover, we derive an analytical expression for the corresponding detection threshold which depends on the statistics of the desired signal from the dedicated TX, the statistics of the MC channel, and the statistics of the ILI. We also provide a low-complexity suboptimal decision threshold. Furthermore, we derive an analytical expression for the bit error rate (BER) and the achievable rate of a single transmission link. Finally, we propose two new performance metrics, namely area rate efficiency (ARE) and area and time rate efficiency (ARTE), suitable for holistically evaluating spatially distributed multi-link MC systems. In particular, ARE and ARTE capture the tradeoff between transmission link density and achievable rate per link and the tradeoff between transmission link density, achievable rate per link, and inter-symbol interference (ISI), respectively. Hence, ARE and ARTE can be exploited to determine the optimal transmission link density for maximizing the throughput of the entire system.

Index Terms—Molecular communication, analytical solution, diffusion, fluid flow, channel impulse response, performance metric, bit error rate.

I. INTRODUCTION

MOLECULAR communication (MC) is a bio-inspired paradigm, in which molecules are used to convey information. It is envisioned that MC is an attractive alternative to electromagnetic wave based wireless communication in challenging environments such as sea water, pipe networks, etc. [2]. However, the practical feasibility of MC and the spectrum of future applications depend on whether it is possible to engineer MC systems achieving high transmission reliability and large data rates. So far, the achievable data rates in MC systems are comparatively low and typically only a single transmission link is considered, i.e., one transmitter (TX) node releases molecules and one receiver (RX) node counts the received molecules. A common approach for increasing the throughput of MC systems is to decrease the symbol duration, which however leads to inter-symbol interference (ISI) [3], [4], [5].

Besides the time dimension, the spatial dimension can be exploited to increase the system throughput. Hereby, choosing an appropriate spatial arrangement enables the efficient usage of this additional degree of freedom for system design. However, this option has received less attention in the MC literature. Existing works exploit the spatial dimension for example in the context of multiple-input multiple-output (MIMO) MC systems [6], [7], [8], [9], [10] or for large-scale MC systems with randomly distributed TXs [11], [12], [13], [14]. A MIMO MC system comprises one TX and one RX, but the TX and the RX are connected to multiple spatially distributed release and reception sites, respectively. Hence, well known techniques such as spatial modulation for encoding [8], [9], and selection combining and zero forcing for decoding [6], [10] are applicable. Performance benefits of MIMO MC systems, such as diversity gain and spatial multiplexing gain, are discussed in [6], [7]. In all existing studies on MIMO MC systems, the considered number of release/reception sites is relatively low. To the best of the authors’ knowledge, the largest system was investigated in [9], which studied an 8 × 8 system. Unlike the studies on MIMO MC, large-scale MC systems with an asymptotically large number of randomly distributed TXs are investigated in [11], [12], [13], [14]. In [11], a swarm of randomly placed TXs simultaneously transmit the same bit sequence to one RX. Methods from stochastic geometry are utilized to analyze the received signal and the corresponding bit error rate (BER). Stochastic geometry is also exploited in [12], where the signal-to-noise ratio and the signal-to-interference ratio

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for randomly distributed MC links are studied for both synchronous and asynchronous TXs. The authors in [13] extend the work of [11], [12] by proposing an interference mitigation method based on error correction coding and a modulation scheme relying on two different types of molecules. In [14], stochastic geometry is applied to study quorum sensing of randomly distributed bacteria. On the other hand, according to [15], [16], the spatial distribution of the bacteria impacts the efficiency of quorum sensing when multiple bacteria-based communication processes take place simultaneously. In this context, a system comprised of multiple different bacteria colonies can be modelled as a multi-link system. In such a system, quorum sensing enables communication within each colony and between different colonies due to the inter-link interference [16, Sec. VII], which facilitates cooperation, parasitism, and competition [17]. The latter is realized by causing intentional interference, i.e., some colonies use enzymes to destroy the quorum sensing signals of other colonies, see [16, Fig. 7] and [18]. In [15], [19], the authors show quantitatively that the interaction of spatially distributed colonies is distance dependent. In fact, in [15] synthetically designed bacteria colonies which are both competitive and cooperative are investigated. Here, cooperation is vital as the colonies possess complementary functions to re-mediate environmental contamination, but they compete for nutrients among the colonies. As shown in [15, Fig. 3], an optimal spatial separation between the colonies exist, which maximizes the viability of the colonies, i.e., a spatial distribution which balances the inter-colony competition and cooperation. These examples highlight the importance of studying the use of the spatial resource and developing performance metrics that allow the evaluation of multi-link MC systems.

In order to gain a fundamental understanding of the benefits of exploiting the spatial dimension for MC, in this paper, we study an MC system with a large number of transmission links, i.e., an asymptotic regime in terms of the number of TX and RX nodes. In contrast to [11], [12], [13], [14], where the TX positions are random, we assume deterministic TX and RX positions, which allows us to reveal the impact of the choice of the TX and RX positions on the performance of the system. We ask the following research question: For given transmit and receive areas, accommodating multiple TXs and RXs, respectively, how densely should the TXs and RXs be deployed to maximize the information transmission rate? Similar to other resources such as transmission time and bandwidth in wireless communication, space is a limited resource, which is valuable in natural multi-link MC systems, and is expected to also become valuable in synthetic systems. Hence, due to being limited, space allocation to different links needs to be optimized. There exists a fundamental tradeoff between the achievable data rate of one TX-RX link, which we refer to as link rate, and the link density. Increasing the density of TXs and RXs increases the number of transmission links per unit area. We refer to the number of links per unit area as spatial multiplexing rate with unit [m⁻²]. However, the molecules released from different TXs may cause inter-link interference (ILI) at the RX units. Therefore, increasing the density of TXs and RXs increases the BER and consequently decreases the link rate. In order to analyze this tradeoff, we propose a new performance metric for multi-link MC systems which we refer to as area rate efficiency (ARE). The ARE is the product of the spatial multiplexing rate and the link rate, and characterizes how efficiently the available TX and RX areas are used for information transmission and is given in terms of bits per unit area.

To systematically address the research question posed above, we study a three-dimensional (3-D) multipoint-to-multipoint MC system comprising multiple non-cooperative, spatially distributed point-to-point transmission links and analyze the system in the asymptotic regime with a large number of TX and RX nodes. As in conventional wireless communications, we define a location model for the positions of the TXs and RXs in the considered multi-link MC setup [20], [21]. For wireless cellular networks, the two most common geometric models for the locations of base stations are fixed hexagonal and random grids, respectively [21]. In both models, the positions of the users are assumed to be random. The authors in [20] show that, for real-world base station locations, one relevant performance metric, namely the signal-to-interference-plus-noise-ratio (SINR) experienced by the users, is upper bounded by the SINR of the users in an idealized grid network, and lower bounded by the SINR of the users in a random network. While existing research on multi-link MC systems is based on randomly positioned TXs and RXs [11], [12], [13], [14], in this work, we assume an idealized, fixed, and predefined grid structure for the TXs and RXs. In particular, the TXs and RXs are arranged on a virtual TX and RX plane, respectively, cf. Fig. 1. Therefore, the model considered in this paper provides a new perspective on multi-link MC systems. We evaluate the performance of the considered system by deriving an analytical expression for the ARE. The main contributions of this work include:

1) An analytical expression for the channel impulse responses (CIRs) of all TX-RX links for multipoint-to-multipoint molecule transmission via diffusion and uniform flow is derived assuming point TXs and cylindrical, transparent RXs.

2) Based on the CIR and a statistical model, mathematical expressions for the optimal detection threshold of a threshold detector, the BER, the link rate, the spatial multiplexing rate, and finally the ARE are derived in the asymptotic regime of a large number of TX-RX links.

3) By analyzing the ARE, we demonstrate a fundamental tradeoff between the spatial multiplexing rate and the ILI dependent link rate on the overall performance of the considered multipoint-to-multipoint transmission system. Our analysis shows that there exists an optimal number of transmission links per unit area which maximizes the ARE. We further show that an optimal link density also exists in the presence of ISI, which is revealed by analyzing an extension of the ARE denoted as area and time rate efficiency (ARTE).

4) We show that the optimal transmission link density, which maximizes the ARE, depends on the number of released molecules and the diffusion coefficient of the molecules. Furthermore, our results reveal that the background noise concentration and the choice of the grid structure have negligible impact on the optimal link density.
The ARE was introduced in the conference version [1] of this paper. Compared to [1], the system model in this paper also accounts for background noise molecules. Furthermore, in addition to the hexagonal grid for the TX and RX positions considered in [1], we also study a square grid. Moreover, a suboptimal threshold based detector is developed, which enables low complexity threshold detection for cases in which the optimal threshold based detector might not be feasible. In addition, the impacts of ISI on the optimal link density is investigated.

The remainder of this paper is organized as follows. Section II introduces the system model and performance metrics for evaluation of the considered multi-link system. In Section III, an analytical expression for the link CIR is derived and a statistical model for the considered MC system is provided. The threshold character of the maximum likelihood detector is unveiled in Section IV, where also the resulting BER is derived. In Section V, the BER and ARE are studied and compared to particle-based and Monte Carlo simulations. Finally, in Section VI, our main conclusions are summarized.

II. SYSTEM MODEL

In this section, we discuss the general arrangement of the MC system, the fixed and predefined grid structure, and the model for modulation, propagation, and reception used in this paper. Moreover, we present different metrics for characterizing the performance of information transmission in the considered system. Hereby, we introduce the ARE as a new performance metric for evaluation of the performance of multi-link MC systems. Finally, extending the definition of the ARE, we define the ARTE as a performance metric for cases, where ISI occurs.

A. General Arrangement

We consider a 3-D unbounded MC environment with an infinite number of point TXs and an infinite number of transparent RXs, cf. Fig. 1. The TXs and RXs are located in the \( xy \)-plane at \( z = z_{\text{TX}} \) and at \( z = z_{\text{RX}} \), respectively. Both planes are virtual (i.e., they are transparent), have infinite width and height (i.e., they extend infinitely in the \( x \) and \( y \) directions), and are placed \( d = z_{\text{TX}} - z_{\text{RX}} \) apart. In the following, these planes are referred to as TX plane and RX plane, respectively. Each TX in the TX plane is paired with the closest RX in the RX plane, i.e., each TX wants to communicate with only one dedicated RX. We denote the individual TXs and RXs as \( \text{TX}_i \) and \( \text{RX}_j \), \( i, j \in \mathbb{N} \), respectively. We note that the number of TXs is equal to the number of RXs. Furthermore, we assume uniform flow in the \( z \) direction with velocity \( v_z \). The chosen setup ensures error-free transmission if only flow is present and impairing factors such as diffusion and noise sources are absent. Of course, due to the use of small-sized molecules, diffusion always occurs in practice. Hence, the random nature of diffusion degrades the performance of the considered transmission links.

The transparent, molecule counting RX model is widely used in the MC literature, see [22], [23], [24], mainly due to its passivity, i.e., such RXs do not impair molecule movement. For complex MC systems, such as the one considered in this work, transparent RXs facilitate the analysis.
wireless communication networks [20], [21]. Furthermore, hexagons are the shape closest to a circle that can form a continuous grid, and therefore, guarantee the densest packing of non-overlapping cells. The square grid is suboptimal in terms of packing, however, it is simple to describe in Cartesian coordinates. The center points of the hexagons and squares of packing, it is simple to describe in Cartesian coordinates.

Fig. 3. The TX positions are shown as black dots within the virtual square grid with the Cartesian coordinate system $x_{\text{cart}}$ and $y_{\text{cart}}$ as axes. The distance $b$ between two adjacent TXs and, as an example, the distance $r_5$ between the reference TX in the center and $TX_5$ are depicted by arrows. Multiple TXs having the same distance to $RX_0$ are conceptually grouped into rings of interferers which are highlighted with the same grid fill color, e.g., the cells of $TX_1 - TX_4$, $TX_5 - TX_{12}$, and $TX_{13} - TX_{24}$ are in green, blue, and orange, respectively. This eases the identification of the structure composed by squares.

C. Modulation, Propagation, and Reception

At the beginning of each symbol interval $l \in \mathbb{N}$, each point $TX_i$ releases a fixed non-zero number of molecules, $N_m$, or zero molecules, representing binary symbols $s_{i,l} = 1$ and $s_{i,l} = 0$, respectively, i.e., the TXs use ON-OFF keying (OOK) modulation [27]. Since the focus of this paper is the spatial dimension, we assume, for now, that ISI is negligible which is a valid assumption if the symbol durations are sufficiently large. Thus, the transmitted symbols are orthogonal in time, and therefore, we omit symbol interval index $l$ in the following. We assume that binary values 0 and 1 are equiprobable, i.e., $\Pr(s_i = 1) = 0.5 = \Pr(s_i = 0)$. The molecules emitted by different TXs are of the same type, and the TXs are synchronized, i.e., they transmit at the same time instants. We assume that molecules do not interact with each other, i.e., the release, propagation, and reception of different molecules are independent, respectively. The propagation of the molecules released by the TXs is affected by diffusion, characterized by diffusion coefficient $D$, and uniform flow in $z$-direction, characterized by flow velocity $v_z$. We neglect additional effects influencing the propagation of molecules such as external forces, turbulences in the flow profile, and degradation. Each transparent RX counts the number of molecules within its volume $V_{RX}$ at a fixed sampling time $t_s$. The sampling time $t_s$ at $RX_0$ is chosen such that it coincides with the time instant where the CIR between $TX_0$ and $RX_0$ has its peak. The RXs are identical cylinders with radius $S_{RX}$ and length $L_{RX}$, i.e., $V_{RX} = \pi S_{RX}^2 L_{RX}$, see Fig. 1. We chose cylindrical receivers as this allows an independent scaling of the structures, the cell center distances $b$ and $c$ are chosen such that the area size of the hexagon cell equals the area size of the square cell, i.e., $A_{\text{hex}} = A_{\text{quad}}$, which is ensured by choosing $b = c \sqrt{\frac{3}{2}}$. The considered arrangement ensures that for $TX_i$, the distance to $RX_j$ is shorter than the distance to any other $TX_j$, $i \neq j$. Moreover, without loss of generality, in the following, we exemplary analyse the point-to-point transmission link between $TX_0$ and $RX_0$, which are both at the origin of the $x$-$y$ plane, see Figs. 2 and 3.

Fig. 3. The TX positions are shown as black dots within the virtual square grid with the Cartesian coordinate system $x_{\text{cart}}$ and $y_{\text{cart}}$ as axes. The distance $b$ between two adjacent TXs and, as an example, the distance $r_5$ between the reference TX in the center and $TX_5$ are depicted by arrows. Multiple TXs having the same distance to $RX_0$ are conceptually grouped into rings of interferers which are highlighted with the same grid fill color, e.g., the cells of $TX_1 - TX_4$, $TX_5 - TX_{12}$, and $TX_{13} - TX_{24}$ are in green, blue, and orange, respectively. This eases the identification of the structure composed by squares.

3Using an offset coordinate system is an approach to uniquely label cells in hexagonal grids by integer tuples of $x', y'$, which simplifies the follow-up geometric analyses, e.g., the derivation of distances. Finally, the results obtained for the offset coordinate system can be related to a different coordinate system, e.g., the Cartesian coordinate system, by coordinate transformation methods.

3Perfect alignment of the transmission and reception sites is an assumption used also in the existing literature on distributed MC systems [9], [25], [26]. In addition, for conventional wireless communication networks, systems where the base stations are organized according to an idealized grid have been shown to provide performance upper bounds for practical wireless cellular systems [20]. Hence, the MC system considered in this work may also provide a performance bound for MC systems with non-aligned TXs and RXs. Proving this conjecture is an interesting topic for future work.

2We note that for some MC systems large symbol intervals may not be optimal for maximizing data throughput, of course. Instead, small symbol intervals may be preferable which leads to ISI. However, including ISI into the system model proposed in this work renders the mathematical analysis infeasible. Thus, we neglect ISI in our analytical work, but provide insight into the impact of ISI based on computer simulations in Section V-D2.

5Time synchronization is a common assumption in the MC literature [9], [14], [25] and can be achieved by adopting existing MC synchronization techniques [28], [29], [30], [31].
receiver size in the $xy$-plane via $S_{\text{RX}}$ and along the $z$-axis via $L_{\text{RX}}$. Furthermore, the circular cross-section of the RX fills both the hexagonal grid and the square grid to a great extent if $S_{\text{RX}}$ is chosen large.

### D. Performance Metrics for Multi-Links MC Systems

In this section, we define the single link rate, the spatial multiplexing rate, and the ARE, for performance evaluation of multi-link MC systems. Finally, we define the ARTE for MC systems employing short symbol intervals such that ISI of multi-link MC systems. Finally, we define the ARTE for multiplexing rate, and the ARE, for performance evaluation.

1) **Link Rate:** We model the point-to-point transmission link as a binary channel with achievable data rate [32, eq. (9.7)]

$$R_{\text{SISO}} = I(s_0; h_0) = H(h_0) - H(h_0 | s_0),$$

as OOK is a binary modulation scheme, i.e., $s_0, h_0 \in \{0, 1\}$. We refer to $R_{\text{SISO}}$ as link rate. $s_0$ and $h_0$ correspond to the channel input symbol and the channel output symbol, respectively, and $I(\cdot)$ and $H(\cdot)$ denote the mutual information and the entropy function, respectively, where [32, eq. (2.35)]

$$H(h_0) = -\frac{1}{2}[(p + q) \log_2(\frac{1}{2} (p + q)) + (q + p) \log_2(\frac{1}{2} (q + p))]$$

and [32, eq. (8.4)]

$$H(s_0 | h_0) = -\frac{1}{2}((p \log_2(p) + p \log_2(p) + q \log_2(q) + (q \log_2(q)) | \{\mathcal{P} = 1 - p\} \text{ and } | \{q = 1 - q\})$$

with $q = \Pr\{s_0 = 0 | s_0 = 1\}$ and $p = \Pr\{s_0 = 1 | s_0 = 0\}$ denote the error probability for $s_0 = 1$ and $s_0 = 0$, respectively.

2) **Spatial Multiplexing Rate:** We define the spatial multiplexing rate $R_{\text{loc}}$ as the number of transmission links per unit area, i.e., $R_{\text{loc}} = \frac{1}{A_{\text{cell}}}$ with unit [m$^{-2}$], where $A_{\text{cell}}$ is the area size reserved for one TX-RX pair, i.e., one hexagon or one square. Hence, the smaller $A_{\text{cell}}$ is, the larger is the spatial multiplexing rate.

3) **Area Rate Efficiency:** We define the ARE based on $R_{\text{SISO}}$ and $R_{\text{loc}}$ as follows

$$\text{ARE} = R_{\text{SISO}} R_{\text{loc}} = \frac{1}{A_{\text{cell}}} [H(h_0) - H(h_0 | s_0)],$$

with unit [bit m$^{-2}$]. Note that the two rates, $R_{\text{SISO}}$ and $R_{\text{loc}}$, exhibit a different dependence on the density of the TXs and RXs. In particular, increasing the density of the TX-RX pairs increases $R_{\text{loc}}$ but decreases $R_{\text{SISO}}$ as the BER increases, and vice versa. Hence, the ARE reflects both the single link performance in terms of $R_{\text{SISO}}$ and the area usage efficiency in terms of $R_{\text{loc}}$. Therefore, the ARE provides a useful performance metric to gain insight into how efficiently given TX and RX areas are exploited for the maximization of the overall information transmission.

4) **Area and Time Rate Efficiency:** We define the ARTE based on $R'_{\text{SISO}}$, $R_{\text{loc}}$, and symbol duration $T_{\text{sym}}$ as follows

$$\text{ARTE} = R'_{\text{SISO}} R_{\text{loc}} \frac{1}{T_{\text{sym}}} = \frac{1}{A_{\text{cell}}} [H(h_0) - H(h_0 | s_0)] \frac{1}{T_{\text{sym}}},$$

with unit [bit m$^{-2}$ s$^{-1}$]. Here, $R'_{\text{SISO}}$ denotes the link rate in the presence of ISI. From (3) we observe that, unlike the ARE, the ARTE incorporates the symbol duration. Hence, the ARTE provides insight into how efficiently the given TX and RX areas are exploited in a given time interval. The ARTE in (3) enables a comprehensive analysis of multi-link MC systems, as both time and area usage in conjunction with the impact of ILI and ISI are considered. However, deriving analytical expressions for the BER and therefore the ARTE for this case appears to be infeasible due to the complex joint ISI and ILI statistics. In fact, the overall interference comprises ISI from TX$_0$, interference from the other TXs, and ISI from the other TXs. Hence, we do not pursue analytical expressions for the ARTE and instead analyze the ARTE based on Monte Carlo simulations in Section V-D2.

To be able to analyze the considered multi-link system in terms of its ARE and ARTE, in the following, we first analyze the relevant MC channels, detection design, and transmission errors, respectively.

### III. ANALYTICAL CHANNEL MODEL

In this section, we first derive an expression for the CIR of all transmission links that involve receiver RX$_0$. We note that the derived CIR expression is also valid for all other TX-RX pairs due to the symmetries in the considered system model. Then, we analyze the distributions of the information, the interfering, and the background noise molecules, respectively.

#### A. Channel Impulse Response

CIR$_t(t)$ denotes the probability to observe one molecule at RX$_0$ at time $t$ which was released by TX$_i$ at position $p_i = (x_{TX_i}, y_{TX_i}, z_{TX_i})$ and at time $t_0 = 0$. In the following proposition, we provide an analytical expression for CIR$_t(t)$ for the considered unbounded environment with constant advection along the $z$-axis with velocity $v_z$ and diffusion coefficient $D$.

**Proposition 1:** The expected number of received molecules at RX$_0$ centered at $(0, 0, z_{RX})$ with radius $S_{RX}$ and extending in $z$-direction from $z_0 = z_{RX} - L_{RX}$ to $z_0 = z_{0} + L_{RX} = 2z_{RX} + \frac{L_{RX}}{2}$, due to the release of one molecule by TX$_i$ at time $t_0 = 0$, is given by

$$\text{CIR}_t(t) = \frac{1}{2} \left( \text{erf} \left( \frac{2z_{TX} + v_z t - z_0}{\sqrt{4Dt}} \right) - \text{erf} \left( \frac{2z_{TX} + v_z t - z_0}{\sqrt{4Dt}} \right) \right) \times \exp \left( -\frac{r_i^2}{4Dt} \right) \sum_{k=0}^{k_{\text{max}}=\infty} \frac{\left( \frac{r_i^2}{4Dt} \right)^k}{(k!)^2} \gamma(k + 1, \frac{z_{RX}^2}{4Dt}),$$

where $r_i^2 = x_{TX_i}^2 + y_{TX_i}^2$, Furthermore, erf$(x)$ and $\gamma(a, x)$ denote the Gaussian error function and the lower incomplete Gamma function, respectively.

**Proof:** Please refer to Appendix A.

Eq. (4) shows that the expected number of molecules received from TX$_i$ depends on the TX position characterized by $r_i$. We observe that CIR$_t(t) \rightarrow 0$ for TXs that are far away from...
RX₀, because, in this case, rᵢ → ∞. All other parameters in (4), e.g., the z-position of the TXs, the diffusion coefficient D, and the flow velocity vₑ are identical for all TXs.

**Proposition 2:** For evaluation of (4), we can ensure that the truncation error for CIRᵢ(tₙᵢ), i > 0, is below a predefined fraction η of CIR₀(t = tₙ₀) when setting k_max to a finite number k_max = k', i.e., for given η there exist k' such that

\[ \text{CIR}_i(t = t_{n_i}) \big|_{k_{\text{max}}=k'} < \eta \text{ CIR}_0(t = t_{n_0}). \tag{5} \]

*Proof:* Please refer to Appendix B.

**B. Statistical Model**

The total number of observed molecules, rₚ, within RX₀ comprises the information conveying molecules originating from TX₀, cₛ, molecules received from other TXs, c_ILI, which constitute IIL, and background noise molecules, cₓ. Hence, the number of observed molecules at sampling time tₛ at RX₀ is given by

\[ rₚ = cₛ + c_ILI + cₓ. \tag{6} \]

We now discuss the underlying models and associated distributions of cₛ, c_ILI, and cₓ.

1) **Information Molecules:** Nₘ information carrying molecules intended for RX₀ are released by TX₀ for signaling s₀ = 1 at time t = 0. At time instant tₛ, each of these molecules is received with probability CIR₀(t = tₙ₀) at RX₀. The expected (non-normalized) number of observed information molecules at sampling time tₛ is given by \( τₛ = Nₘ \text{ CIR}_0(tₛ) \). We model the received particle statistics by a Poisson distribution, i.e.,

\[ cₛ \sim \text{Pois}(s₀τₛ) = fₛ(cₛ \mid s₀), \tag{7} \]

which is a valid approximation for molecule counting RXs if the number of released molecules is large [27]. Here, \( fₛ(cₛ \mid s₀) \) denotes the distribution of cₛ conditioned on s₀.

2) **Interference Molecules From Other Transmitters:** Besides the information molecules, molecules emitted by TX₁, TX₂, TX₃, ..., TXₙₜₓ₋¹, i.e., the TXs belonging to other TX-RX pairs, are received as IIL at RX₀, where \( Nₜₓ \rightarrow ∞ \) denotes the number of transmitters. Due to the infinite extent of the TX plane, infinitely many interferers exist in principle. We assume that the interfering molecules are not distinguishable from the information molecules. Hence, IIL degrades the detection of the signal of TX₀ at RX₀ [3]. We note that TXᵢ, i ≠ 0, causes interference at RX₀ only for sᵢ = 1 as no molecules are released for sᵢ = 0. Hence, in addition to the Brownian motion of the molecules, the random transmit sequence at TXᵢ introduces randomness into the received signal. So, for a comprehensive statistical analysis, the joint statistics of the transmit sequence at all TXs as well as the statistics of the molecule movement have to be taken into account.

From the perspective of RX₀, the expected number of received molecules at sampling time t = tₛ can be collected in vector \( \overline{c_ILI} = [\overline{c_ILI}_1, \overline{c_ILI}_2, ..., \overline{c_ILI}_{nₜₓ-1}] \) with \( \overline{c_ILI} = Nₘ \text{ CIR}_0(t = tₛ) \), assuming molecule releases at all interferers. Similar to (7), the received number of molecules from each interferer can be characterized by a Poisson distribution [27], as the molecule releases of the different TXs are independent of each other. As RX₀ counts all molecules, independent of their origin, the sum over all Poisson distributed interfering molecules follows again a Poisson distribution, i.e.,

\[ c_ILI \sim \text{Pois}(s_ILI_1^T c_ILI) = f_ILI(c_ILI \mid s_ILI), \tag{8} \]

where \( f_ILI(c_ILI \mid s_ILI) \) denotes the distribution of c_ILI conditioned on vector s_ILI, which contains the symbols emitted by the interfering TXs, i.e., s_ILI = \([s₁, s₂, ..., s_{nₜₓ-1}]\). There are \( Nₘ \times 2^{|nₜₓ|-1} \) possible realizations of s_ILI, i.e., different IIL states, which are equiprobable due to the equiprobable binary transmission symbols. Hence, \( Nₘ \times 2^{|nₜₓ|-1} \) grows exponentially in \( Nₜₓ \) and we assumed \( Nₜₓ \rightarrow ∞ \) in our system model. However, the IIL can be accurately approximated by truncating \( Nₜₓ \) to a finite number, i.e., by taking into account only a finite number of interfering TXs. The IIL is mainly characterized by the strongest interferers, which correspond to the TXs closest to TX₀, as will be confirmed via simulations in Section V-B2. As can be observed from Fig. 2, the indices of the TXs are chosen such that, for increasing index i, the distance between TX₀ and TXᵢ is monotonically non-decreasing in i. Therefore, the strongest interferers are always included if \( Nₜₓ \) is truncated to a finite number. We note that the actual number of TXs necessary to accurately approximate the system behavior depends on the values of the system parameters, see Section V-C.

3) **Background Noise Molecules:** Besides information molecules and molecules from interfering TXs, we also account for background noise molecules, which are of the same type as the signaling molecules. These molecules may originate from far away noise sources. We assume that these molecules are uniformly distributed in space with constant concentration \( C_{\text{noise}} \). We statistically model the reception of the background noise molecules by a Poisson distribution, i.e.,

\[ cₓ \sim \text{Pois}(cₓ) = fₓ(cₓ), \tag{9} \]

which is a valid approximation based on the law of rare events [27]. Here, \( fₓ(cₓ) \) denotes the distribution of cₓ, and \( cₓ \) is given by \( cₓ = C_{\text{noise}} V_{RX} \).

**IV. SYMBOL DETECTION AND BER PERFORMANCE ANALYSIS**

In this section, we derive the optimal maximum likelihood (ML) decision rule and the BER of one TX-RX pair.

**A. Optimal ML Detector**

For detection, we assume all CIRs in the system are known but the activity of the interfering TXs is only statistically

Note that for TX₀, \( r₀ = 0 \) follows and CIR₀(t = tₙ₀) = \( \frac{1}{2} \text{erf}(\frac{tₙ₀+Lₑₙ₀−\overline{h}_//=\sqrt{2D}}{\sqrt{2D}})−\text{erf}(\frac{tₙ₀+Lₑₙ₀−\overline{h}_//=\sqrt{2D}}{\sqrt{2D}})(1−\exp(−\frac{Sₘ^2}{4D})) \) can be evaluated exactly.
known. Therefore, the ML estimate, \( \hat{s}_0 \), is given by

\[
\hat{s}_0 = \arg\max_{s_0 \in \{0, 1\}} f_{T^*}(r_T | s_0) = \arg\max_{s_0 \in \{0, 1\}} \mathbb{E} \{ f_{T^*}(r_T | s_0, s_{\text{ILI}}) \} 
\]

\[
= \arg\max_{s_0 \in \{0, 1\}} \sum_{s_{\text{ILI}} \in \mathcal{M}} f_{T^*}(r_T | s_0, s_{\text{ILI}}) f_{s_{\text{ILI}}}(s_{\text{ILI}}) \tag{10}
\]

\[
= \begin{cases} 
1, & \text{if } \sum_{s_{\text{ILI}} \in \mathcal{M}} f_{T^*}(r_T | s_0, s_{\text{ILI}}) f_{s_{\text{ILI}}}(s_{\text{ILI}}) \geq 1 \\
0, & \text{otherwise}
\end{cases}
\]

\[
= \begin{cases} 
1, & \text{if } \sum_{s_{\text{ILI}} \in \mathcal{M}} (\tau_s + s_{\text{ILI}} \tau_{\text{ILI}}^T + \tau_n)^T \Phi (-\tau_s + s_{\text{ILI}} \tau_{\text{ILI}}^T + \tau_n) \geq 1 \\
0, & \text{otherwise}
\end{cases}
\tag{11}
\]

where \( f_{T^*}(r_T | s_0) \) denotes the distribution of \( r_T \) in (6) conditioned on \( s_0 \), which is a Poisson distribution with mean \( s_0 \tau_r + s_{\text{ILI}} \tau_{\text{ILI}}^T + \tau_n \) as \( \tau_r \), \( \tau_{\text{ILI}} \), and \( \tau_n \) are all Poisson distributed, cf. (7) – (9). Here, \( f_{s_{\text{ILI}}}(s_{\text{ILI}}) \), \( \Phi \{ \cdot \} \), and \( \mathcal{M} = \{0, 1\}^{N_{\text{TX}}-1} \) denote the joint distribution of the transmit symbols of the interferers, the expectation with respect to (w.r.t.) \( s_{\text{ILI}} \), and the set of all possible interference symbol vectors \( s_{\text{ILI}} \), respectively. The ML decision rule in (11) is computationally complex as all possible realizations of the ILI have to be taken into account and (11) has to be computed for every received \( r_T \). Note that evaluating (11) is only feasible for a finite number of interferers, cf. discussion in Section III-B2.

In the following, we show that (11) can be equivalently realized by a multi-threshold detector employing a set of pre-calculated threshold values. The threshold values specify the limits of decision regions, where each region corresponds to either \( s_0 = 1 \) or \( s_0 = 0 \). In principle, for complicated probability distributions \( f_{T^*}(r_T | s_0) \), many regions, and thus many thresholds, are needed. However, we later show in Corollary 1 that for special cases the number of thresholds required reduces to a single threshold. Threshold detection is preferable to (11) as the threshold for a given setup can be computed offline and can then be used throughout the transmission. Therefore, the computational cost for online data detection is reduced.

**Lemma 1**: The ML decision rule given in (11) can be written equivalently as a multi-threshold detection where the finite set of threshold values \( T \), with \( [\Phi] \in T \) and \( \Phi \in \mathbb{R}_+^M \), are obtained as the solutions of the following equation

\[
\sum_{s_{\text{ILI}} \in \mathcal{M}} (\tau_s + s_{\text{ILI}} \tau_{\text{ILI}}^T + \tau_n)^T \Phi (-\tau_s + s_{\text{ILI}} \tau_{\text{ILI}}^T + \tau_n) = \sum_{s_{\text{ILI}} \in \mathcal{M}} (s_{\text{ILI}} \tau_{\text{ILI}}^T + \tau_n)^T \Phi (-s_{\text{ILI}} \tau_{\text{ILI}}^T + \tau_n), \tag{12}
\]

**Proof**: The number of obtained threshold values is finite if \( N_{\text{TX}} \) is truncated to a finite number according to Section III-B2, i.e., \( |T| < \infty \), where \( | \cdot | \) denotes the cardinality of a set. \( |T| \) is upper bounded by the cardinality of \( \mathcal{M} \), i.e., \( |\mathcal{M}| = 2^{N_{\text{TX}}-1} \), which is the number of possible maxima of the distributions in (12). Due to the symmetry in the proposed TX/RX grids, some of the interferers have identical statistical impact on RX0. Therefore, \( |T| < 2^{N_{\text{TX}}-1} \) follows in general.

**Corollary 1**: If \( \frac{\tau_s}{\tau_{\text{ILI}}^T + \tau_n} = \text{SINR}_{\text{worst}} > 1 \), where 1 denotes the \( (N_{\text{TX}} - 1) \)-dimensional all-ones row vector, the ML decision rule given in (11) can be equivalently written as a single threshold detection as follows

\[
\hat{s}_0 = \begin{cases} 
1, & \text{if } r_T \geq \xi_{\text{opt}, N_{\text{TX}}-1}, \\
0, & \text{otherwise}
\end{cases} \tag{13}
\]

with threshold value \( \xi_{\text{opt}, N_{\text{TX}}-1} \) obtained as

\[
\xi_{\text{opt}, N_{\text{TX}}-1} = \min \{ \xi \in \mathbb{N} | \sum_{s_{\text{ILI}} \in \mathcal{M}} (\tau_s + s_{\text{ILI}} \tau_{\text{ILI}}^T + \tau_n)^T \Phi (-\tau_s + s_{\text{ILI}} \tau_{\text{ILI}}^T + \tau_n) \geq \sum_{s_{\text{ILI}} \in \mathcal{M}} (s_{\text{ILI}} \tau_{\text{ILI}}^T + \tau_n)^T \Phi (-s_{\text{ILI}} \tau_{\text{ILI}}^T + \tau_n) \} \tag{14}
\]

**Proof**: Please refer to Appendix D.

Here, \( \text{SINR}_{\text{worst}} > 1 \) is a sufficient, but not a necessary condition. This means that if the condition does not hold, i.e., \( \text{SINR}_{\text{worst}} \leq 1 \), detection based on a single threshold may still be equivalent to the ML decision rule in (11), cf. Lemma 1, but we cannot guarantee this mathematically. However, for all numerical results shown in this work, we have observed equivalence between (12) and (14), i.e., we observed \( |T| = 1 \) for all considered system settings. A simplified but suboptimal decision threshold is obtained by neglecting the randomness of the ILI. In this case, the threshold value is obtained using the mean of \( \tau_{\text{ILI}} \) instead of the actual distribution of the ILI. Therefore, the decision rule in (11) simplifies to

\[
\hat{s}_{0,\text{sub}} = \begin{cases} 
1, & \text{if } \frac{(\tau_s + 0.5 \tau_{\text{ILI}}^T + \tau_n)^T \Phi (-\tau_s + 0.5 \tau_{\text{ILI}}^T + \tau_n) \geq 1,} \\
0, & \text{otherwise}
\end{cases} \tag{15}
\]

Similar to (13), (15) can be equivalently written as a threshold detection scheme with threshold [33, eq. (5)]

\[
\xi_{\text{sub}, N_{\text{TX}}-1} = \frac{\tau_s}{\ln (1 + \frac{\tau_s}{0.5 \tau_{\text{ILI}} + \tau_n})} \tag{16}
\]

**Proof**: We note that the suboptimal threshold in (16) approximately approximates (14) for the extreme case of a large number of non-distinguishable interference signals at RX0, which corresponds to a scenario of densely packed transmission links. In such a scenario, it is sufficient to consider the average ILI. We compare the performance of the detector based on the decision thresholds derived in (14) and (16) in Section V-C3.

### B. BER for One TX-RX Pair

The BER for one TX-RX link can be expressed as follows

\[
P_e = \mathbb{E}_{s_0} \left\{ \mathbb{E}_{s_{\text{ILI}}} \{ P_e(s_0 | s_{\text{ILI}}, s_0) \} \right\} = \sum_{s_0} \sum_{s_{\text{ILI}}} P_e(s_0 | s_{\text{ILI}}, s_0) f_{s_{\text{ILI}}}(s_{\text{ILI}}) f_{s_0}(s_0) \tag{17}
\]
where \( f_{s_0}(s_0) \) and \( P_e(s_0|s_{ILI}, s_0) \) denote the distribution of \( s_0 \) and the error probability conditioned on both the transmitted symbol \( s_0 \) and interference vector \( s_{ILI} \), respectively. In the following, we derive the BER for the detector based on the decision thresholds proposed in (14) and (16).

**Proposition 3:** For the proposed threshold detectors, \( P_e \) can be expressed as follows

\[
P_e = \begin{cases} 
\frac{1}{2} \left( Q(\xi', \tau_s + \tau_n) + (1 - Q(\xi', \tau_n)) \right), & \text{if } N_{TX} = 1 \\
\frac{1}{2} \left( \frac{1}{N_{TX} - 1} \sum_{s_{ILI} \in M} Q(\xi', \tau_s + s_{ILI} \tau_{ILI}^T + \tau_n) \right) + \frac{1}{N_{TX} - 1} \sum_{s_{ILI} \in M} \left( 1 - Q(\xi', s_{ILI} \tau_{ILI}^T + \tau_n) \right), & \text{else}
\end{cases}
\]

where \( \xi' = \xi_{opt}, N_{TX} - 1 \) and \( \xi' = \xi_{sub}, N_{TX} - 1 \) when the decision thresholds in (14) and (16) are used, respectively. Here, \( Q(a, b) \) denotes the regularized Gamma function.

**Proof:** Please refer to Appendix E.

The obtained error probabilities \( p \) and \( q \) can now be used to calculate the link rate and, subsequently, the ARE and ARTE in (1), (2), and (3), respectively. Hence, the proposed multi-link system can be evaluated in terms of the performance metrics introduced in Section II-D.

V. PERFORMANCE EVALUATION

In this section, we first specify the simulation setup. Then, we evaluate the analytical expression for the CIR in (4) and compare it to results from particle-based simulation (PBS). Subsequently, the analytical expressions for the BER in (18b), the ARE in (2), and the ARTE in (3) are evaluated.

A. Simulation Parameters

The default values of the channel parameters are given in Table I and are used if not specified otherwise. Micro-scale parameter values are chosen similar to other MC works [9], [25]. We emphasize that, by default, \( S_{RX} \) is chosen to be as large as possible, such that the RX touches the cell boundary, i.e., \( S_{RX} = \frac{a}{c} \) and \( S_{IL} = \frac{b}{c} \) for the hexagonal and the square grid, respectively. Furthermore, we adopt the hexagonal grid as the default structure. For the evaluation of the CIR, the infinite sum in (4) was truncated to 21 terms, \(^9\) i.e., \( \eta_{\text{max}} = 20 \). Furthermore, the threshold value \( \xi_{opt}, N_{TX} - 1 \) in (14), the suboptimal threshold value \( \xi_{sub}, N_{TX} - 1 \) in (16), and the BER in (18b) were computed for a truncated number of interferers. The numbers of interferers, corresponding to the first three rings in the respective grid, cf. Figs. 2 and 3, i.e., \( N_{TX} - 1 = 36 \) and \( N_{TX} - 1 = 24 \) for the hexagonal and square grids, respectively.

\(^9\) The corresponding mismatch error is bounded by factor \( \eta \) given in Table I, cf. Appendix B.

---

1) **Monte Carlo Simulation:** To validate the analytical expressions for the BER and ARE, and to verify that limiting the number of interferers for numerical evaluation does not affect the accuracy of our analysis, we used Monte Carlo simulation. For Monte Carlo simulation, we considered \( N_{TX} - 1 = 1260 \) and \( N_{TX} - 1 = 840 \) interferers for the hexagonal and square grids, respectively. First, we randomly generated up to \( I = 5 \times 10^5 \) realizations of possible transmit symbol vectors \( s_{all} = [s_0, s_{ILI}] \). Then, we generated the number of molecules observed at RX\( _0 \) based on the channel model in (6), where the random variables \( c_s \) and \( c_{ILI} \) were modeled as Poisson distributed according to (7) and (8). Parameters \( \tau_s \) and \( \tau_{ILI} \) were obtained from the CIR in (4). For Section V-D, the additional ISI part \( c_{ISI} \) was modeled as Poisson distributed as proposed in [34, eq. (1)]. In particular, here the \( c_{ISI} \) takes into account the interfering symbols from both TX\(_0\) and the interfering transmission links. Next, (18b) was numerically evaluated to determine the BER for all possible threshold values up to 100, i.e., \( \xi \leq 100 \), and the lowest BER together with the corresponding threshold value and error probabilities \( p \) and \( q \) were selected.

2) **Particle-Based Simulation:** To verify the accuracy of the analytical expressions for the CIR in (4), 3-D stochastic PBS were carried out [35]. In the PBSs, the signaling molecules propagate in a three-dimensional open space environment and are affected by both uniform flow and diffusion. The results from PBS were averaged over 3000 realizations.

B. Evaluation of CIR and ILI Truncation

1) **Verification of CIR:** Figs. 4 and 5 show the CIR obtained from the proposed analytical expression (4) (black) and PBS for cylindrical RXs (red) as ground truth. Additionally, PBS results for spherical RXs (yellow) are shown as reference. The radius of the spherical RXs, \( S_{RX, Sphere} \), is chosen such that the volume sizes of the cylindrical and the spherical RXs are identical, which leads to \( S_{RX, Sphere} = 2.289 \times 10^{-6} \) m. Here, the CIR of TX\(_0\) can be directly
We first concentrate on the CIRs for default diffusion coefficient $D = 6 \times 10^{-11} \text{m}^2 \text{s}^{-1}$. From Fig. 4, we observe that for the desired transmitter $TX_0$, the proposed CIR is in excellent agreement with the PBS results. For $TX_1$ and $TX_{13}$, (4) deviates from the PBS result for $k_{\text{max}} = 0$, but both match for $k_{\text{max}} = 1$, i.e., for truncating the infinite sum to two terms.\footnote{Note that only for these results, which are based on severe truncation to $k_{\text{max}} = 0$ and $k_{\text{max}} = 1$, the truncation error factor is larger than $\eta = 10^{-6}$.}
We observe a large similarity between the results obtained for $TX_0$ and $TX_1$. For $TX_{13}$, the UCA based CIR approximates (4) well. In general, the expression for CIR$_{\text{UCA,i}}$ is more compact than (4), but less accurate. These observations are also valid for the CIRs for $D = 6 \times 10^{-10} \text{m}^2 \text{s}^{-1}$, which are shown in Fig. 5. Furthermore, by comparing Figs. 4 and 5, we observe that the deviation between CIR$_{\text{UCA,i}}$ and the PBS result is small for larger diffusion coefficients. For small $D$, the spread of the spatial distribution of the released molecules does not significantly change during molecule transport which is mainly determined by flow. As we assume a point release at the TX, i.e., a spatially concentrated molecule distribution, the gradient of the molecule concentration within the receiver volume is large for small diffusion coefficients and contradicts the assumptions underlying the UCA [27]. We observe that the peak CIR value for $TX_0$ decreases when $D$ is increased, as in this case, molecules spread out more during propagation. Finally, we conclude that the derived expression for the CIR in (4) is accurate and in perfect agreement with the ground truth results from PBSs shown in red color. Additionally, we observe a large similarity between the results obtained for cylindrical and spherical RXs, respectively. From this we conclude that our results on the exploitation of the spatial resource, shown in the following, generalize to systems with spherical RXs. Moreover, to get accurate results, visual examination suggests that it may be sufficient to take into account only two terms in the infinite sum in (4) for the parameters considered in Figs. 4 and 5. Nevertheless, we use $k_{\text{max}} = 20$ for

\begin{table}
\centering
\caption{Default Parameter Values}
\begin{tabular}{|c|c|}
\hline
Variable & Definition & Value \\
\hline
$c$ & Cell centers distance in hexagonal grid & $4 \times 10^{-6} \text{m}$ \\
$b$ & Cell centers distance in square grid & $c \sqrt{3} / 2$ \\
$S_{\text{RX}}$ & Receiver radius (neighboring RXs touch each other) & $\frac{c}{2} \& \frac{c}{4}$ in hexagonal \& square grid, respectively \\
$L_{\text{RX}}$ & Receiver length & $4 \times 10^{-6} \text{m}$ \\
$d$ & Distance between TX and RX plane & $1 \times 10^{-5} \text{m}$ \\
$v_s$ & Flow velocity & $6 \times 10^{-6} \text{m} \text{s}^{-1}$ \\
$D$ & Diffusion coefficient & $6 \times 10^{-11} \text{m}^2 \text{s}^{-1}$ \\
$N_m$ & Number of released molecules & 100 \\
$C_{\text{noise}}$ & Background noise concentration & $0 \text{m}^{-3}$ \\
$\Delta t$ & Time step PBS \& Monte Carlo simulation & $10^{-4} \text{s}$ \\
$T_{\text{sim}}$ & Simulation time & 1 s \\
$\eta$ & Maximum truncation error factor in (4) & $10^{-6}$ \\
\hline
\end{tabular}
\end{table}

\begin{figure}
\centering
\includegraphics[width=0.5\textwidth]{fig5}
\caption{CIR from (4) for $TX_0$ (solid black) and for $TX_1$ and $TX_{13}$ (dashed black) realized by a truncation of the sum in (4) to $k_{\text{max}} = 0$ and $k_{\text{max}} = 1$. The UCA based CIR deviates from the PBS result, especially for $TX_0$ and $TX_1$. For $TX_{13}$, the UCA based CIR approximates (4) well. In general, the expression for CIR$_{\text{UCA,i}}$ is more compact than (4), but less accurate. These observations are also valid for the CIRs for $D = 6 \times 10^{-10} \text{m}^2 \text{s}^{-1}$, which are shown in Fig. 5. Furthermore, by comparing Figs. 4 and 5, we observe that the deviation between CIR$_{\text{UCA,i}}$ and the PBS result is small for larger diffusion coefficients. For small $D$, the spread of the spatial distribution of the released molecules does not significantly change during molecule transport which is mainly determined by flow. As we assume a point release at the TX, i.e., a spatially concentrated molecule distribution, the gradient of the molecule concentration within the receiver volume is large for small diffusion coefficients and contradicts the assumptions underlying the UCA [27]. We observe that the peak CIR value for $TX_0$ decreases when $D$ is increased, as in this case, molecules spread out more during propagation. Finally, we conclude that the derived expression for the CIR in (4) is accurate and in perfect agreement with the ground truth results from PBSs shown in red color. Additionally, we observe a large similarity between the results obtained for cylindrical and spherical RXs, respectively. From this we conclude that our results on the exploitation of the spatial resource, shown in the following, generalize to systems with spherical RXs. Moreover, to get accurate results, visual examination suggests that it may be sufficient to take into account only two terms in the infinite sum in (4) for the parameters considered in Figs. 4 and 5. Nevertheless, we use $k_{\text{max}} = 20$ for

\footnote{Note that only these results, which are based on severe truncation to $k_{\text{max}} = 0$ and $k_{\text{max}} = 1$, the truncation error factor is larger than $\eta = 10^{-6}$, while for all other results, which are based on $k_{\text{max}} = 20$, $\eta = 10^{-6}$ holds.}}
by using a larger or smaller threshold value compared to \( \xi_{opt,N\_TX-1} \), i.e., \( \xi > \xi_{opt,N\_TX-1} \) or \( \xi < \xi_{opt,N\_TX-1} \), respectively, increases the BER. We further observe from Fig. 6 that truncating the number of interferers to a smaller value can result in a lower threshold value, i.e., \( \xi_{opt,6} \leq \xi_{opt,18} \leq \xi_{opt,36} \leq \xi_{opt,1260} \), and a lower BER. Thus, if the number of interferers considered is not sufficient, a threshold deviation results, i.e., \( \xi_{opt,1260} > \xi_{opt,6} > 0 \), which leads to a BER degradation.\(^{12}\) The deviation of the threshold value as well as the subsequent performance loss in terms of the BER are depicted in Fig. 6. From Fig. 6, we further observe a close match between the BER results for \( N_{\_TX} = 1 = 36 \) and the baseline case, while there exists a mismatch between the BER results for \( N_{\_TX} = 1 = 18 \) and the baseline case. Hence, the ILI from more than 18 additional transmission links notably impairs the link between TX0 and RX0, which leads to the obtained larger BER. We finally conclude that truncating the number of interferers to \( N_{\_TX} = 1 = 36 \) is sufficient for \( c = 4 \times 10^{-6} \) m.

In Fig. 7, the agreement between the baseline case and the result obtained by truncation of the number of interferers to \( N_{\_TX} = 1 = 6 \) is excellent. Thus, for \( c = 4 \times 10^{-6} \) m, \( N_{\_TX} = 1 = 6 \) is sufficient to accurately model the impact of ILI. Note that here condition (25) is satisfied as \( \text{SINR}_{\text{worst}} = \{1.726913, 1.717973, 1.717973, 1.717973\} \) for \( N_{\_TX} = 1 = \{6, 18, 36, 1260\} \), respectively.

The exact number of interferers required to accurately estimate the optimal threshold value \( \xi_{opt,\infty} \) for the system depends on the system parameters and should be chosen carefully. A simple method to obtain the necessary number of interferers is by brute force search, i.e., iteratively increasing \( N_{\_TX} \) and evaluating the BER until the increase results in a non-distinguishable change of the BER. In particular, we verify this brute force method by additionally showing performance results for \( N_{\_TX} = 1 = 1260 \) interferers for comparison in Figs. 8–13. Hence, as long as the results for 36 and 1260 interferers are identical, 36 interferers are sufficient to characterize the entire ILI. Note that the results in Section V-C for \( N_{\_TX} = 1 = 36 \) interferers are obtained analytically from (14), (18b), and (2), while the results for \( N_{\_TX} = 1 = 1260 \) interferers are obtained by Monte Carlo simulations, if not specified otherwise. The reason for utilizing Monte Carlo simulation for large numbers of interferers is that for 1260 interferers, the analytical evaluation of the results becomes infeasible due to the \( 2^{N_{\_TX}} \) possible realizations of the interference term, which need to be considered, i.e., \( \approx 6.9 \times 10^{10} \) vs. \( \approx 2 \times 10^{379} \). Finally, we observe from Figs. 6 and 7 that the achievable BER for \( c = 4 \times 10^{-6} \) m is about one order of magnitude smaller than that for \( c = 4 \times 10^{-5} \) m. This is intuitive as the ILI decreases for increasing \( c \) and therefore the BER decreases.

\(^{12}\) The setup, which considers six interfering transmitting links, can also be interpreted as a system of small extent. Since grid size is kept constant, due to the reduced ILI, such system results in a smaller BER, as expected, cf. Section II-B.
C. Evaluation of BER, ARE, and ARTE

In this section, we evaluate the BER, ARE, and ARTE for various scenarios.

1) Impact of Background Noise on BER and ARE:

Figs. 8 and 9 depict the BER and ARE as functions of the hexagonal cell center distance \( c \) for different background noise molecule concentrations \( C_{\text{noise}} \). We observe from Fig. 8 that BER approaches 0.5 for small \( c \) and for increasing \( c \), the BER decreases in the absence of background noise molecules. However, for \( C_{\text{noise}} > 0 \), above a certain value of \( c \), the BER increases again (see green and cyan curves). In fact, if a certain cell center distance \( c \) with corresponding cell area \( A_{\text{cell}} \) is exceeded, a further increase leads to a larger number of received background noise molecules, but not to a larger number of received information carrying molecules, which causes the BER to increase. Furthermore, as expected, the BER increases for increasing number of background noise molecules.

Fig. 9 shows that the ARE has a unique maximum and we denote the corresponding cell center distance as \( c_{\text{opt}} \). We observe that both, decreasing and increasing \( c \) compared to \( c_{\text{opt}} \), decreases the simulated ARE asymptotically to \( \text{ARE} \to 0 \).

For small \( c \), the considered system suffers from excessive ILI, i.e., the resulting small \( R_{\text{SISO}} \) mainly limits the ARE in (2). However, for large \( c \), the system’s usage of the spatial resource is not optimal, as the hexagonal cell area reserved for one TX-RX link is large, and the small \( R_{\text{SISO}} \) limits the ARE in (2). From the existence of a maximum ARE, we conclude that there exists an optimal TX-RX link density, which is achieved by TX positions with cell center distance \( c = c_{\text{opt}} \). We further observe that the maximum ARE decreases for increasing background noise molecule concentration. We note that \( c_{\text{opt}} \) and therefore, the optimal TX-RX link density shows no dependency on the background noise molecule concentration.

Finally, we observe from Fig. 9, that the analytical ARE (2) deviates from the Monte Carlo simulation result for small \( c \). The reason for this is that the actual number of interferers needed to accurately approximate the system behavior increases with decreasing \( c \). Hence, for small \( c \), more than 36 interferers have to be considered in order to properly model the ILI.

2) Hexagonal Grid vs. Square Grid: In this section, we investigate the impact of the type of grid, diffusion, and flow velocity on BER and ARE. As discussed in Section II, we assume equal cell area sizes, i.e., \( A_{\text{hex}} = A_{\text{quad}} = b^2 \). Furthermore, the RX radius \( S_{\text{RX}} \) is chosen such that neighboring RXs touch, but do not overlap. As a consequence, \( S_{\text{RX}} \) and therefore the RX volumes are smaller for the square grid compared to the hexagonal grid, i.e., \( S_{\text{RX,hex}} > S_{\text{RX,quad}} \), and consequently \( V_{\text{RX,hex}} > V_{\text{RX,quad}} \).

In Figs. 10 and 11, BER and ARE are shown as a function of the cell area \( A_{\text{cell}} \) for the two considered grids, hexagonal and square, and different diffusion coefficients \( D \). The results from Monte Carlo simulation are depicted by markers.
As the number of observed interfering molecules increases at the sampling time decreases and simultaneously, for increasing $D$, the number of information molecules observed at the sampling time decreases and simultaneously the number of observed interfering molecules increases at $R X_0$. In Fig. 11, we observe that the peak of the ARE is higher for smaller $D$ and is obtained for a smaller cell area $A_{\text{cell}}^{\text{opt}}$. We further observe that the flow-free scenario yields a larger BER and smaller ARE compared to the scenario with $v = 6 \times 10^{-5} \text{ m s}^{-1}$. Finally, Figs. 10 and 11 show that for the flow-free scenario varying the diffusion coefficient yields unaltered results. This is intuitive, as for this scenario a change in $D$ has no impact on the number of information molecules observed at the peak time, which itself may change.

Next, we consider the effect of the chosen grid structure. We observe from Fig. 10 that the BER for the hexagonal grid is lower than that for the square grid. Furthermore, Fig. 11 shows a higher maximum ARE for the hexagonal grid than for the square grid. Hence, the hexagonal grid is preferable compared to the square grid in terms of BER and ARE. However, the performance differences between both grid structures are small and diminish for large values of $A_{\text{cell}}$. Finally, we observe from Fig. 11 that the analytical results deviate from the Monte Carlo simulations for very small $A_{\text{cell}}$ as in this case not enough interferers are taken into account.

3) Comparison of Methods to Derive the Threshold Value:
In this section, we evaluate the loss in performance caused by the suboptimal threshold value $\xi_{\text{sub},N_{TX}-1}$ in (16). We further show the impact of the number of released molecules $N_m$ on the BER and ARE.

Figs. 12 and 13 show that for small cell center distances $c$, the BER and ARE results for $\xi_{\text{opt},N_{TX}-1}$ and $\xi_{\text{sub},N_{TX}-1}$ are indistinguishable because of the excessive interference. In particular, for small $c$, more interferers are relevant and the individual interferers are positioned close to each other and therefore have a similar impact on the information transmission of $TX_0$, as the amount of interference is distance-dependent. Hence, for small $c$ an averaging effect occurs, and employing the suboptimal threshold $\xi_{\text{sub},N_{TX}-1}$, which neglects the higher-order ILI statistics, is sufficient. Next, we observe that for increasing $c$, which corresponds to moderate ILI, the usage of $\xi_{\text{sub},N_{TX}-1}$ for detection compared to $\xi_{\text{opt},N_{TX}-1}$ leads to a higher BER and consequently to lower ARE values. We further observe that the ARE degradation increases with increasing $N_m$.

Next, we focus on the impact of the numbers of released molecules $N_m$ on the BER and ARE. In Fig. 12, we observe that for increasing $N_m$ the BER decreases. Fig. 13 shows that increasing $N_m$ also increases the peak value of the ARE. We observe that $c_{\text{opt}}$ is smaller for larger numbers of released molecules $N_m$, i.e., the optimal density of the independent transmission links is larger for larger $N_m$. In particular, $N_m$ linearly scales $\tau_b$, cf. Section III-B1. Hence, the difference...
between \( s_0 = 1 \) and \( s_0 = 0 \) w.r.t. the expected number of received molecules, i.e., \( \mathbb{E}(r_T | s_0 = 1) - \mathbb{E}(r_T | s_0 = 0) \), increases with increasing \( N_m \), and therefore improves the performance of the threshold based detection. In practical applications, however, there might be an upper limit for \( N_m \) due to limited resources.

From this section, we conclude that, as expected, detection with threshold \( \xi_{\text{opt}, N_{TX} - 1} \) yields a higher performance than with \( \xi_{\text{sub}, N_{TX} - 1} \). However, the loss in terms of BER and ARE is small and diminishes for some system settings, such as small numbers of released molecules \( N_m \).

### D. Impact of the Symbol Duration on BER and ARE

In this section, we show the ARE as defined in (3) for various symbol durations. As small symbol durations lead to ISI, we also show results obtained by utilizing appropriate equalizers proposed for MC [34], which mitigate the ISI.

1) **Design of the Equalizers:** We evaluate the BER and ARTE for two linear equalization schemes, namely a linear symbol rate (SR)-equalizer and a linear fractionally spaced (LFS)-equalizer [34], and compare them to a scheme without equalization. Here, the equalizers use \( L \times M \) samples of the received signal, where \( L \) and \( M \) denote the number of considered symbols and the samples per symbol, respectively. In particular, \((L - 1)/2 \times M\) samples are obtained before \( t_0\), one sample at \( t_0\), and \((L + 1)/2 \times M - 1\) samples after \( t_0\). The samples are spaced uniformly by \( T_{\text{sym}}/M\). For the SR-equalizer \( M = 1 \) is used by definition. A general mathematical expression for the output signal of the linear equalizers can be found in [34, eq. (4)]. Here, for each considered value of \( c\), the value of \( T_{\text{sym}} \) is chosen such that the ARTE is maximized for the two depicted equalization schemes, i.e., an increase and decrease of \( T_{\text{sym}} \) to larger and lower values, respectively, results in lower ARTEs.

2) **Simulation Results Considering ILL and ISI:**

Figs. 14 and 15 depict the BER and the ARTE, respectively, as functions of the hexagonal cell center distance \( c\), the symbol duration \( T_{\text{sym}}\), and the equalization scheme. Additionally, the BER and \( c_{\text{opt, ISI-free}}\) of the ISI-free scenario are shown for reference.

Fig. 14 shows a BER of 0.5 for small \( c\), which decreases for increasing \( c\), similarly to all previously shown BER results. However, above a certain value of \( c\) the BER increases again. This behavior is caused by an increase of the ISI. In particular, as \( c\) increases, the RX volume increases. Therefore, molecules of symbols previously sent by \( TX_0\) are more likely to be observed in the current symbol interval. A further increase in \( c\) results in a constant error floor. As for large \( c\) the ILL approaches zero, the level of the error floor is mainly ISI dependent. From Fig. 14, we observe that for increasing symbol duration \( T_{\text{sym}}\) the BER decreases. This is intuitive as an increase in \( T_{\text{sym}}\) decreases the ISI and therefore improves the information transmission performance.

Next, we compare the performance of the different equalization schemes in Fig. 14. In accordance with [34], the LFS-equalizer achieves the best performance, i.e., the lowest BER, followed by the SR-equalizer, except for \( T_{\text{sym}} = 0.2\) s. Furthermore, as expected, the scheme which does not perform equalization, exhibits the largest BER, again with the exception of \( T_{\text{sym}} = 0.2\) s. In particular, for \( T_{\text{sym}} = 0.2\) s, the BERs obtained with the SR-equalizer and without equalization are similar, while the results obtained with the LFS-equalizer are worse. From this, we conclude that for \( T_{\text{sym}} \geq 0.2\) s the BER performance degradation caused by ISI is small. In contrast, for \( T_{\text{sym}} < 0.2\) s, ISI deteriorates the performance as is evident from the comparison with the ISI-free scenario (solid black line), which assumes very long symbol durations.

The computations of the equalization filter coefficients require the inversion of the covariance matrix of the received signal, which becomes numerically unstable if the determinant of the matrix approaches zero. The numerical instability, which is more critical for the LFS-equalizer, is the reason for the worse performance of the LFS-equalizer compared to the SR-equalizer for \( T_{\text{sym}} = 0.2\) s.

---

13) In [36], frequency domain equalizers for MC systems are proposed. Additionally, the authors of [34] investigate non-linear fractionally spaced decision feedback (FSDF)-equalizers, whose BER performance was shown to be similar to that of LFS-equalizers for the MC scenarios considered in [34]. To avoid overcrowding Figs. 14 and 15, we only include results for linear equalization schemes. However, we note that more sophisticated equalizers can yield improved BER and ARTE performance.
From Fig. 15, we observe that even in the presence of ISI the ARTE exhibits a unique maximum w.r.t. the cell center distance \( c \), which is achieved for \( c_{\text{opt}} \). However, \( c_{\text{opt}} \) depends on both the symbol duration \( T_{\text{sym}} \) and the equalization scheme. Fig. 15 shows that the highest ARTEs are achieved by the LFS-equalizer, followed by the SR-equalizer, and the scheme without equalization. This is intuitive, as the equalizers mitigate the ISI and improve the BER (cf. Fig. 14), while the other factors in (3), namely \( T_{\text{sym}} \) and \( \frac{1}{T_{\text{sym}}} \), are independent of the choice of equalizer. Again, as in Fig. 14, \( T_{\text{sym}} = 0.2 \) s is an exception. In particular, for \( T_{\text{sym}} = 0.2 \) s, no equalizer and the SR-equalizer, the optimal cell center distance equals the one of the ISI-free scenario, i.e., \( c_{\text{opt}}, T_{\text{sym}} = 0.2 \) s = \( c_{\text{opt,ISI-free}} \). The LFS-equalizer performs worse due to its inferior BER performance. From these observations, we conclude that, for the given parameter values, \( T_{\text{sym}} = 0.2 \) s is a sufficiently large symbol duration for which ISI can be neglected.

Next, we concentrate on the impact of \( T_{\text{sym}} \) for the scheme without equalization. Fig. 15 shows that the largest ARTE is reached for \( T_{\text{sym}} = 0.08 \) s at a cell center distance \( c_{\text{opt}}, T_{\text{sym}}=0.08 \) s. We observe that decreasing the symbol duration \( T_{\text{sym}} \) changes \( c_{\text{opt}} \) and decreases the maximum ARTE. In particular, for \( T_{\text{sym}} = 0.04 \) s and \( T_{\text{sym}} = 0.016 \) s it is optimal w.r.t. the overall ARTE to employ smaller cell areas compared to \( T_{\text{sym}} = 0.08 \) s, while for \( T_{\text{sym}} = 0.01 \) s larger areas are favorable. The observed non-linear dependence of the ARTE on \( T_{\text{sym}} \) emphasizes the importance of the analysis presented here. Next, we compare the symbol durations \( T_{\text{sym,max}} \), which yield the largest ARTEs for the considered schemes. We observe that an increase in the number of samples utilized by the equalizer improves its ability to handle interference and therefore can decrease \( T_{\text{sym,max}} \) as well as \( c_{\text{opt}} \). In particular, \( T_{\text{sym,max}} = 0.08 \) s, \( T_{\text{sym,max}} = 0.08 \) s, and \( T_{\text{sym,max}} = 0.016 \) s for the scheme without an equalizer, the SR-equalizer, and the LFS-equalizer, respectively. We note that for large cell center distances \( c \), \( T_{\text{sym}} = 0.08 \) s yields the highest ARTEs despite the significant ISI.

We observe that neither the largest nor the smallest symbol durations and cell center distances yield the maximum ARTE. Hence, to optimize information transmission in a multi-link MC system, i.e., to reach the maximum ARTE, both \( T_{\text{sym}} \) and \( c \) should be judiciously chosen. Finally, we observe from Fig. 15 that cell center distance \( c_{\text{opt,ISI-free}} \), which maximizes the ARE, is close to the optimal cell center distances in the ISI impaired scenarios. Hence, by analyzing and optimizing the ARE, which is computationally feasible, a cell center distance which incurs a small performance loss in terms of the ARTE compared to the optimal cell center distance can be found.

VI. CONCLUSION

In this paper, we focused on the spatial dimension of MC systems. We considered a 3-D system with multiple independent and spatially distributed point-to-point transmission links, where the TXs and the RXs were positioned according to a regular grid pattern. We proposed the ARE and ARTE as new performance metrics for MC systems to characterize how efficiently given TX and RX areas are utilized for information transmission. Since space is a valuable resource in multi-link MC scenarios, the ARE and ARTE are relevant performance metrics. To evaluate the considered system in terms of its ARE, we developed analytical expressions for the CIRs of all existing TX-RX links, the optimal and suboptimal threshold values for detection, and the BER of a single transmission link. Finally, we obtained quantitative results for the optimal spatial link density maximizing the ARE of MC systems. We showed that the maximum ARE is strongly dependent on the number of released molecules and the concentration of the background noise, whereas the considered grid and the approximation error in the calculation of the threshold value have only a minor impact on the maximum ARE. Furthermore, we revealed that the optimal link density depends on the number of released molecules and the diffusion coefficient. On the other hand, our obtained results showed that the background noise concentration and the grid structure have a negligible impact on the optimal link density.

In this paper, we have analyzed the ARE and ARTE for a specific MC system under idealized assumptions used such as perfect alignment of TXs and RXs, perfect time synchronization, uniform flow, and transparent RXs. These assumptions can be relaxed in future work to extend the analysis of the ARE and ARTE to different MC channels, unsynchronized transmission, more realistic RX models, e.g., absorbing RXs [37], and different TX and RX location models including random location models.

APPENDIX A

DERIVATION OF THE CIR

The molecule concentration \( C(x, \bar{x}_{\text{TX}}, y, y_{\text{TX}}, z, z_{\text{TX}}, t, t_0) \) at position \( (x, y, z) \) for the case considered in Proposition 1, i.e., transmitter position \( p_i = (\bar{x}_{\text{TX}}, y_{\text{TX}}, z_{\text{TX}}) \) and release time \( t_0 = 0 \), is given in [27, eq. (18)]. \( C(x, \bar{x}_{\text{TX}}, y, y_{\text{TX}}, z, z_{\text{TX}}, t, t_0) \) can be transformed to a cylindrical coordinate system by \( x = r \cos(\varphi), y = r \sin(\varphi), \bar{x}_{\text{TX}} = r \cos(\varphi_1), y_{\text{TX}} = r \sin(\varphi_1) \). Here, \( \varphi \) denotes the angle in the \( xy \)-plane in relation to the positive \( x \)-axis. We obtain:

\[
C(r, r_1, \varphi, \varphi_1, z, z_{\text{TX}}, t) = \frac{1}{(4\pi D t)^{3/2}} \times \exp\left(\frac{-r^2 + r_1^2 - 2r_1 r \cos(\varphi - \varphi_1) + (z - z_{\text{TX}} - v_2 t)^2}{4 D t}\right).
\]

(19)

Furthermore, since the center of the circular cross-section of RX\(_0\) is located at \( r = 0 \), the expected number of counted molecules is obtained as

\[
\text{CIR}_i(t) = \int_0^{S_{\text{RX}}} 2\pi z \int_0^{\frac{S_{\text{RX}}}{2\pi}} C(r, r_1, \varphi, \varphi_1, z, z_{\text{TX}}, t) r \, dz \, d\varphi \, dr
\]

\[
= \left(\frac{1}{4 D t}\right)^{3/2}(\text{erf}(m_0) - \text{erf}(m_1))
\]

\[
\times \int_0^{S_{\text{RX}}} \int_0^{\frac{r_1 \pi}{2 D t}} I_0\left(\frac{r_1 r}{2 D t}\right) \exp\left(-\frac{r^2 + r_1^2}{4 D t}\right) r \, dr
\]

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where we substituted 

\[ m_0 = \frac{x + q_1 - \sqrt{E}}{\sqrt{D_1 t_0}} \quad \text{and} \quad m_1 = \frac{x + q_2 - \sqrt{E}}{\sqrt{D_1 t_0}} \]

and exploited (a) \( \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-y^2) \, dy \) \( \text{and} \) \( I_0(x) = \frac{1}{\pi} \int_0^\infty \exp(x \cos(\varphi)) \, d\varphi \), (b) the series expansion of \( I_0(x) \) \[ \text{(38, eq. (9.6.10))}, \] (c) the relation between the Gamma function and the factorial \( \Gamma(n) = (n-1)! \). Finally, we exploit \( \gamma(a, x) = \int_0^x y^{a-1} \exp(-y) \, dy \) to obtain (4). Here, \( I_0(x) \) denotes the zeroth order modified Bessel function of the first kind.

**APPENDIX B**

**PROOF OF THE MISMATCH ERROR BOUND OF THE CIR FOR FINITE \( k_{\text{max}} \)**

The bound of the mismatch error \( \text{CIR}_k(t = t_0) \big|_{k_{\text{max}} = \infty} - \text{CIR}_k(t = t_0) \big|_{k_{\text{max}} = k'} \) is obtained as

\[
\text{CIR}_k(t = t_0) \big|_{k_{\text{max}} = \infty} - \text{CIR}_k(t = t_0) \big|_{k_{\text{max}} = k'} = \frac{1}{2} \left( \text{erf} \left( \frac{x + q_1 - \sqrt{E}}{\sqrt{D_1 t_0}} \right) - \text{erf} \left( \frac{x + q_2 - \sqrt{E}}{\sqrt{D_1 t_0}} \right) \right) \times \exp \left( -\frac{r^2}{4D_1 t_0} \right) \sum_{k'=k+1}^{k_{\text{max}}} \frac{\left( \frac{r^2}{4D_1 t_0} \right)^k}{k!} \gamma(k+1, w_3) \Gamma(k+1) \]

\[(a) \quad w_0 w_1 \sum_{k=k'+1}^{k_{\text{max}}} \frac{w_2}{k!} \Gamma(k+1) \Gamma(k+1) \]

\[(b) \quad w_0 w_1 \sum_{k=k'+1}^{k_{\text{max}}} \frac{w_2}{k!} (1 - \exp(-w_3))^{k+1} \]

\[(c) \quad w_0 w_1 (1 - \exp(-w_3)) \sum_{k=k'+1}^{k_{\text{max}}} \frac{(w_2 - w_2 \exp(-w_3))^k}{k!} \]

\[(d) \quad w_5 \left( \sum_{k=0}^{\infty} \frac{w_4^k}{k!} - \sum_{k=0}^{k'} \frac{w_4^k}{k!} \right) \]

\[(e) \quad w_5 \left( \exp(w_4) - \exp(w_4) \frac{\Gamma(k' + 1, w_4)}{\Gamma(k' + 1)} \right) \]

\[(f) \quad w_5 \exp(w_4) \frac{\Gamma(k' + 1, w_4)}{k!} \gamma(k' + 1, w_4) \leq \eta \quad \text{CIR}_0(t = t_0) \quad \text{(21)} \]

where we substitute in (a) \( w_0 = \frac{1}{2} \left( \text{erf} \left( \frac{x + q_1 - \sqrt{E}}{\sqrt{D_1 t_0}} \right) - \text{erf} \left( \frac{x + q_2 - \sqrt{E}}{\sqrt{D_1 t_0}} \right) \right) \) \( \text{and} \) \( x = \exp(-\frac{r^2}{4D_1 t_0}) \), (b) \( \frac{w_4}{k!} \), (c) \( \frac{(w_2 - w_2 \exp(-w_3))^k}{k!} \), (d) \( \frac{w_4^k}{k!} \), (e) \( \exp(w_4) \frac{\Gamma(k' + 1, w_4)}{\Gamma(k' + 1)} \), and (f) \( \gamma(k' + 1, w_4) \).}

**APPENDIX C**

**PROOF OF LEMMA 2**

Rearranging (22) yields \( \gamma(z, x) (1 - \exp(-x))^z \leq \Gamma(z) \), for which equality holds for \( x \to \infty \). Therefore, to prove Lemma 2, it is sufficient to show that \( f_2(x) = \gamma(z, x) (1 - \exp(-x))^z \) is monotonically increasing in \( x \), given \( x > 0 \) and \( z > 1 \), i.e.,

\[
\frac{\partial}{\partial x} f_2(x) = \exp(\gamma(z, x) (1 - \exp(-x))^z - 1) \leq 0. \]

Since \( \exp(\gamma(z, x) (1 - \exp(-x))^z - 1) > 0 \), we need to show that \( g_2(x) = \gamma(z, x) (1 - \exp(-x))^z - \int_0^x y^{z-1} \exp(-y) \, dy > 0 \), which is achieved by showing that \( g_2(0) = 0 \) and \( \frac{\partial}{\partial x} g_2(x) = (z-1)x^{z-2} \exp(-x)(1 - x) > 0 \) for \( x > 0 \). In fact, \( x^{z-2} \exp(-x) > 0 \) for \( z > 1 \) and \( x > 0 \). Furthermore, \( \exp(x) > 1 + x \) holds as \( \exp(x) = x + x^2/2 + \cdots \). This concludes the proof.

**APPENDIX D**

**PROOF OF EXISTENCE OF OPTIMAL THRESHOLD VALUE**

The existence of a unique threshold level \( \xi_{\text{opt}, N_{TX}} \) can be proven by showing that the ratio in (11) is monotonically increasing in \( \rho_1 \), i.e., for low values of \( \rho_1 \), i.e., \( \rho_1 < \xi_{\text{opt}, N_{TX}} \), the fraction is always smaller than 1, and for large values of \( \rho_1 \), i.e., \( \rho_1 > \xi_{\text{opt}, N_{TX}} \), the fraction is always at least equal to 1. This can be proven using the same steps as in a similar proof in [33, Appendix].

**Lemma 3:** If function \( f_1(t) \) is monotonically increasing, then function \( \sum_{i=0}^{\infty} g_i(t) \) is also monotonically increasing.

**Proof:** Please refer to the proof in [33, Appendix].

For Lemma 3, we have to show that

\[
f_1(t) = \left( \tau_5 + s_{t_{\text{LL}}} \frac{\tau_{t_{\text{LL}}} + \tau_5}{\tau_{t_{\text{LL}}} + \tau_5} \right) \frac{\tau_{t_{\text{LL}}} + \tau_5}{\tau_{t_{\text{LL}}} + \tau_5} \exp \left( -\left( \tau_5 + s_{t_{\text{LL}}} \frac{\tau_{t_{\text{LL}}} + \tau_5}{\tau_{t_{\text{LL}}} + \tau_5} \right) \right) \]

\[
\text{and} \quad g_i(t) = \left( \tau_5 + s_{t_{\text{LL}}} \frac{\tau_{t_{\text{LL}}} + \tau_5}{\tau_{t_{\text{LL}}} + \tau_5} \right) \frac{\tau_{t_{\text{LL}}} + \tau_5}{\tau_{t_{\text{LL}}} + \tau_5} \exp \left( -\left( \tau_5 + s_{t_{\text{LL}}} \frac{\tau_{t_{\text{LL}}} + \tau_5}{\tau_{t_{\text{LL}}} + \tau_5} \right) \right) \times \exp(\cdots) \exp(s_{t_{\text{LL}}} \frac{\tau_{t_{\text{LL}}} + \tau_5}{\tau_{t_{\text{LL}}} + \tau_5}) \]

\[(24) \]

\[
\text{and} \quad g_i(t) = \left( \tau_5 + s_{t_{\text{LL}}} \frac{\tau_{t_{\text{LL}}} + \tau_5}{\tau_{t_{\text{LL}}} + \tau_5} \right) \frac{\tau_{t_{\text{LL}}} + \tau_5}{\tau_{t_{\text{LL}}} + \tau_5} \exp \left( -\left( \tau_5 + s_{t_{\text{LL}}} \frac{\tau_{t_{\text{LL}}} + \tau_5}{\tau_{t_{\text{LL}}} + \tau_5} \right) \right) \times \exp(\cdots) \exp(s_{t_{\text{LL}}} \frac{\tau_{t_{\text{LL}}} + \tau_5}{\tau_{t_{\text{LL}}} + \tau_5}) \]

\[(24) \]
is monotonically increasing in $r_T$ for all combinations of $l$ and $p$, where $s_{III,l}$ and $s_{III,l,p}$ denote two possible realizations of $s_{III}$. Therefore, as long as

$$\sum_{s_{III,l,p}} \frac{1}{s_{III,l,p}} \frac{\sum_{r_T} r_T \{ r_T < \xi' | s_{III,l} = 0 \}}{\sum_{r_T} r_T \{ r_T \geq \xi' | s_{III,l} = 0 \}} \geq \frac{\sum_{r_T} r_T \{ r_T < \xi' | s_{III,l} = 0 \}}{\sum_{r_T} r_T \{ r_T \geq \xi' | s_{III,l} = 0 \}}$$

(25) is valid, the existence of a unique threshold value can be guaranteed, where $1$ denotes the all-ones row vector. Note that $\text{SINR}_{\text{worst}} > 1$ is a sufficient, but not a necessary condition, i.e., for $\text{SINR}_{\text{worst}} \leq 1$, a single threshold value might still be equivalent to the ML decision rule given in (11). However, this can not be guaranteed.\(^15\)

### APPENDIX E

**DERIVATION OF THE BIT ERROR RATE**

The BER $P_e$ in the presence of ILI, i.e., $N_{TX} > 1$ can be derived as follows:

$$P_e = \frac{1}{2N_{TX}-1} \sum_{s_{III,l} \in M} \left( \frac{1}{2} P_T \{ r_T < \xi' | s_{III,l, \xi_0} = 1 \} + \frac{1}{2} P Т \{ r_T \geq \xi' | s_{III,l, \xi_0} = 0 \} \right)$$

(26) where we exploit in (a) the threshold detection rule (13), in (b) the fact that $r_T$ is an integer value, and in (c) the mass function property $\sum_{r_T} f(r_T) = 1$ and the fact that $r_T$ is Poisson distributed. Finally, we exploit $\sum_{k=0}^{x-1} (\lambda^k e^{-\lambda}) / k! = Q(x, \lambda)$, with $x > 0$ to obtain (18b). Here, $\Gamma(a,b) = Q(a,b)$ denotes the regularized Gamma function. In the absence of ILI, i.e., $N_{TX} = 1$, (18b) simplifies to (18b).

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\(^{15}\) A similar proof was given in [33, Appendix]. Contrary to the statement there, $\frac{f(r_T)}{g(r_T)}$ is not always a monotonically increasing function in $r_T$. However, imposing the mild condition $\min\{\tau_a\}/\max\{\tau_b\} > 1$ (i.e., the worst-case signal-to-noise ratio (SNR) is larger than 0 dB) guarantees the monotonicity of $\frac{f(r_T)}{g(r_T)}$ in $r_T$ and the rest of the proof remains valid.
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