Stochastic Modelling of Dynein Motors in One-Dimensional Lattice: Simulation and Mean Field Analysis

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Abstract. We introduce a one-dimensional non-equilibrium lattice gas model variant, to represent the motion of dynein molecular motors over the microtubule. We study both dynamical and stationary state properties for the model that consists of hardcore particles hopping on the lattice with varying step size. In our numerical simulation, we find that the stationary state gap-distribution shows striking peaks around gap sizes that are multiples of the maximum hop distance ($m_s$), for both open and periodic boundary conditions. We have verified the presence of these peaks using a mean-field calculation. Further, in the case of open boundary conditions, we observe the intriguing damped oscillator-like distribution of particles over the lattice where the wavelength of these oscillations is multiple of the maximum hop distance. To characterize transient dynamics, we measure the mean square displacement that shows weak superdiffusive growth with exponent $\gamma \sim 1.35$ for periodic boundary and ballistic growth ($\gamma \sim 2$) in case of open boundary conditions at early times.
1. Introduction

Biological molecular motors are protein molecules that transport molecular cargos within the living cells by moving progressively along actin filaments and microtubules [1, 2]. The term “motor” is motivated by the fact that molecular motors utilize the chemical energy produced by the hydrolysis of ATP (Adenosine triphosphate) to ADP (Adenosine diphosphate) to perform mechanical work. This progressive movement of motors is often considered as analogous to the traffic in a city, where the cytoskeletal filaments act as the path along which the molecular motors travel in a directed fashion [3]. The efficient transport of molecular motors is critical for the healthy functioning of a cell as they play crucial roles in many biological processes such as cell division, transfer of genetic information, etc. Therefore, understanding the motor dynamics constitutes an important and relevant research area. Among the three known motor families, kinesins and dyneins move along a microtubule, whereas myosins move on an actin filament [4]. Unlike the other two, cytoplasmic dynein mediates retrograde transport shuttling organelles, vesicles, etc. from the edge to the body of the cell. Owing to several experiments and theoretical modeling of the dynamics of motors in the last few years, we have a reasonably good understanding of the mechanism of processive backward/forward motion of kinesin and myosin. However, the functioning of cytoplasmic dynein is much less understood. Advancement in probing techniques in recent years have shed some light on the structural complexity and motility of dynein motors. Moreover, experimental studies of dynein have shown that they exhibit an unusual gear-like mechanism taking variable step sizes of 8, 16, 24, and 32 nm depending on the concentration of ATPs available and external loads [5, 6].

Motivated by this jump strategy with variable step-size, in this paper we introduce a simple one-dimensional stochastic model, with the goal to understand the effect of this motility mechanism on the collective dynein dynamics. Both analytical and numerical stochastic modeling of statistical physics is predominantly used to understand wide varieties of biological phenomena ranging from transport to cell division [7, 8, 9, 10]. For such studies, particle-based modeling [11] constitutes a simplified, idealized but powerful approach where one ignores the structural complexity of individual biological motors and considers them as hardcore particles that jump (move) across lattice sites (linear microtubule tracks). The process of hydrolysis is a constant source of energy to the motors, which can be represented in the model as a constant driving force for the particles. Such a driving force prevents the system from ever relaxing to thermal equilibrium. Thus, after an initial transient period of non-equilibrium dynamics, the system asymptotically evolves to a non-equilibrium stationary state [7]. In 1968, a very simple one-dimensional model, the totally asymmetric simple exclusion process (TASEP), was first used to model the collective movement of ribosomes on messenger RNA track [12]. Later TASEP variants were introduced to study molecular motors [8]; however, very few of the earlier studies are based on dynein motors [13, 14, 15]. To understand the collective behavior of dynein motors, specifically, how dyneins optimize step sizes depending on different parameters such as loads and the presence of the other motors [15, 16], we formulate a TASEP variant. In this approximate model of dynein transport, which incorporates the essential load-dependent hopping mechanism, we investigate their long-time as well as the transient time behavior. Although open boundary conditions represent a more realistic model for a system of biological motors, we decide to study the system with periodic boundary conditions first since the bulk properties of the system are not affected by this choice. Later we look at the boundary effects by simulating our model with open boundary conditions. We find that the stationary-state gap distribution in front of the motors exhibit intriguing peaks at multiples of the maximum jump size, with the amplitude of these peaks decaying exponentially as function of the gap size.
For open boundary conditions, we observe a damped oscillatory density profile starting from the entry sites. Depending on the influx and escape rates and the rates of attachment/detachment, these oscillations decay as one moves further into the bulk leading to a flat density profile. We also analyze the superdiffusive growth of the mean square displacement during the transient time followed by standard diffusive behavior.

This paper is structured as follows: In the following section, we describe our stochastic model and review the known gear-like jump mechanism of dynein motors. We then discuss the results for the static and dynamics of the model for periodic boundary conditions in Section 3.1. Section 3.2 is devoted to the discussion of the properties of the model for open boundary conditions. We conclude with a summary of our results and open questions in Sec. 4.

2. Model and Simulation Method

In this section, we briefly review the structure and the mechanism of motion of dynein motors; we refer the reader to Ref. [5] for a detailed description. Cytoplasmic dynein performs unidirectional discrete jumps on the microtubule. Structurally, a dynein motor has two heads; each head contains 6 AAA (ATPases Associated with diverse cellular Activities) domains, four of which are potentially ATP binding sites, as shown in Fig. 1. Earlier studies of dynein motors show that the hydrolysis (conversion of ATP to ADP) occurs on all ATP binding sites; however, only the hydrolysis at the primary site AAA1 is compulsory for the movement of the motors, so the motors do not hop until the primary site hydrolyzes. The attached ATP units on secondary sites act as an external load for the motors, which determine the step size and also influence other molecular functions [6, 15].

In our study, we introduce a variant of the totally asymmetric exclusion process to model the dynamics of dynein motors. We consider $L$ discrete lattice sites with $N$ hardcore particles which we refer to as $N$-motor system. A lattice site can be occupied by at most one particle, and each particle jumps in the forward direction with varying step sizes of 1, 2, 3 or 4 depending on the number of ATP units attached to the secondary sites (loads) of the particle. Each particle carries a flag for
Figure 2: Transport of dynein motors on a lattice with periodic boundary conditions (left) and with open boundary conditions (right). For open boundary conditions, motors enter and exit the lattice with influx and escape rates $\alpha$ and $\beta$, respectively. Motors hop forward (clockwise) $n$ steps with rate $v_n$ and $m$ ($m > n$) empty sites in front of them.

the occupancy of one primary and three secondary ATP binding sites. Additionally, we also assume that there is an infinite source of ATP units available for binding. We employ random sequential Monte-Carlo update where, at each time step of the simulation, a motor is chosen randomly from an occupied lattice site. The hopping probability with varying step size is determined by three distinct processes:

ATP attachment- One unit of ATP attaches to the empty primary site with probability $P_{on}$ or to any of the available secondary sites, with probability $S_{on}$.

ATP detachment- One unit of ATP detaches either from the primary or one of the three secondary sites with probabilities $P_{off}$ and $S_{off}$, respectively.

ATP hydrolysis- A filled primary binding site hydrolyzes and converts ATP to ADP. This chemical reaction leads to energy production, which propels the motor forward. The number of steps the motor moves depends on the number of ATP units bound to the secondary sites and the number of available empty lattice sites in front of the motor. If the secondary ATP binding sites are unoccupied, the motor attempts to hop to the maximum step size of four. If $s$ number of secondary sites hold ATP ($s$ can be 1, 2, or 3), given the primary binding site is occupied, the motor attempts to hop $(4 - s)$ steps. The motor can only take a step forward as long as there is no other motor blocking its path. If $n$ is the attempted hopping size and $m$ is the number of empty lattice sites in front of the motor, it takes $\min(m, n)$ steps. In actual biological motors, even the secondary sites hydrolyze ATP to ADP, but this does not result in forward propulsion of the motor. In our $N$-motor system, secondary site hydrolysis is not considered. However, one can argue that the detachment rate of AAA(2-4) takes care of the hydrolysis of ATP from secondary sites.

The stochastic probabilities of attachment and detachment $P_{on}$, $S_{on}$, $P_{off}$, $S_{off}$ are in general considered to be functions of the stall force, the temperature of the cellular environment and other physical parameters [6]. For simplicity, we choose constant rates in our study. Furthermore, experimental observations suggest that the attachment rate of ATP to the primary site is large.
in comparison to the ATP attachment rate to secondary sites inside the living cells. Thus, we will present most of our results for high attachment rates to AAA1, and for the case when, $S_{on} = 1 - P_{on}$, $P_{off} = 1 - P_{on}$, $S_{off} = P_{on}$. All simulation results are obtained for lattice size $L = 10^3$ for periodic boundary conditions and $L = 500$ for open boundary conditions. Ensemble averaging of $10^4$ different realizations has been performed for all final results.

Thus, for maximum possible step-size $m_s$, the hopping rate of particle is given by

$$u_n(m) = \sum_{i=1}^{m_s-1} \delta_{m,i} \sum_{j=1}^{i} v_j \delta_{n,j} + \theta(m - m_s) \sum_{i=1}^{m_s} v_i \delta_{n,i},$$

(1)

where $v_n$ is a function of the attachment and detachment rates chosen in the simulation for step size $n$, and the delta function puts a constraint on the step size due to $m$ empty lattice sites in front of the motor. Here, we aim to understand the effect of various rates of attachment/detachment, and of the motor density on the fluctuations and stationary state properties of the system. We have studied the system for both periodic and open boundary conditions shown in Fig. 2. For open boundary conditions the same dynamical rules of hopping apply in the bulk as for the periodic boundary case. Moreover, the open ends of the lattice are attached to a reservoir through which a motor can enter and exit with the rates $\alpha$ and $\beta$ from the first and last site, respectively.

3. Results

3.1. Periodic Boundary Conditions

3.1.1. Steady-state properties: We solve for the stationary state properties of the system. Ignoring higher-order correlations, we can define the mean-field particle current as

$$j(\rho) = \sum_{i=1}^{m_s-1} \rho [a_i \sum_{j=1}^{i} (1 - \rho)^j],$$

(2)

where $a_i$ is the rate of hopping $i$ steps. For the limiting case of $P_{on} = S_{off} = 1$, $S_{on} = P_{off} = 0$, only the rate $a_4$ is non-zero implying that the particle always tries to hop four steps. The expression for the current simplifies to,

$$j(\rho) = a_4 \rho \sum_{i=1}^{4} (1 - \rho)^i.$$

For this limiting case, one can easily check that the maximum current is obtained at density $\rho_{max} = 0.33$. The current profile obtained in simulation for $P_{on} = 1$ indeed peaks at a $\rho \sim 0.33$ as can be seen from Fig. 3(a). We observe that the maxima of the current is obtained for densities below $\rho = 0.5$ for all our chosen rates. This shift signifies the absence of particle-hole symmetry and suggests the self-assembly of particles and holes to optimize the jump efficiency. To validate this claim, we observe the load current $L(\rho)$ which is the measure of the total amount of “load” or ATP transported by the secondary sites. For $P_{on} = 0.8$, this quantity attains maximum value at $\rho \sim 0.4$ which is only slightly different from the peak of the density versus current plot, see inset of Fig. 3(a). Setting $S_{on}$ equal to zero, and $m_s$ to one, we recover the well-known TASEP results [11].

To understand this self-organization of the particles, we investigate the distribution of particle clusters as well as the distribution of empty spaces in front of the particles referred to as gap distribution, $P(m)$. In the stationary state, the particle cluster is Poisson distributed for all choices
Figure 3: (a) Current profile $j(\rho)$ as a function of density for four different rates of attachment and detachment. The numerically obtained data points (red points) are compared with the mean-field Eq. 2 (black line) for $P_{on} = 1$, the maximum current is obtained at $\rho = 0.33$. Inset shows efficiency of load transport $L(\rho)$ maximizes at density $\rho \sim 0.4$ for $P_{on} = 0.8$. (b) The distribution of the hop sizes performed by the motors in the stationary state peaks at hope size four for all densities. Attachment and detachment rates used in the simulation are $P_{on} = S_{off} = 0.8$, $P_{off} = S_{on} = 0.2$.

of rates at all densities, as shown in Fig. 4(a). The characteristic size of the cluster depends not only on the density but also on the chosen rates of attachment and detachment. One can also extract the correlation length from the slopes for the log-linear plot of cluster distribution. We find that the correlation length of the system increases exponentially with density of particles. Moreover, the gap distribution shows a very striking feature for our specific choice of $P_{on}$, $S_{on}$, $P_{off}$, and $S_{off}$. The distribution peaks at multiples of the maximum possible step size $m_s$, and the amplitude of the peaks decay exponentially for large $m$, as can be seen in the inset of Fig. 4(b). We inspected this further by simulating the gap distribution for various $m_s$, and the characteristic features of the peaks observed are consistent. These peaks signify that the motors assemble themselves in such a way that they optimize the utilization of energy by taking the maximum possible jump lengths. This observation is supported by the step-size distribution plot 3(b) as well, where one can see the particles indeed prefer to hop the maximum length of four steps rather than to shorter steps of one, two or three for all range of densities. We also notice that the step size distribution of four steps peaks at density $\rho \approx 0.3$.

In order to analytically calculate the gap distribution in the mean-field approximation, we write the time evolution equation for the probability of finding a gap of size $m$ for a totally biased
Stochastic Modelling of Dynein Motors in One-Dimensional Lattice

walk in the following form \[13, 17, 18\]:

\[
\frac{dP(m,t)}{dt} = \left[ \sum_{k=1}^{m} u_k(m) + \sum_{j=1}^{\infty} P(j,t) \sum_{k=1}^{j} u_k(j) \right] P(m,t) + \sum_{k=1}^{m} P(m+k,t) u_k(m+k)
\]
\[
+ \sum_{k=1}^{m} P(m-k,t) \sum_{j=k}^{\infty} P(j,t) u_k(j) \quad (m \geq 1),
\]

\[ (3) \]

\[
\frac{dP(0,t)}{dt} = -P(0,t) \sum_{j=1}^{\infty} P(j,t) \sum_{k=1}^{j} u_k(j) + \sum_{j=1}^{m_s} P(j,t) \sum_{k=1}^{j} u_k(j).
\]

\[ (4) \]

The above equations must satisfy conservation rule of probability and density of the empty space, implying

\[
\sum_{m \geq 0} P(m,t) = 1,
\]

\[ (5) \]

\[
\sum_{m \geq 1} P(m,t) = \frac{1}{\rho} - 1,
\]

\[ (6) \]

where \( \rho = N/L \) is the density of motors present in the system. To handle the infinite set of equations (4), we rewrite it into a single differential equation using the generating function technique where we multiply both sides of Eq. (4) by \( z^m \), sum over all \( m \geq 1 \), and define the generating function \( G(z,t) = \sum_{m \geq 1} z^m P(m,t) \). For the case of \( m_s = 4 \), the further calculation becomes cumbersome. Hence we carry out the analysis for a smaller step size \( m_s = 2 \) and arrive at the simplified form

\[
G(z,t) = \sum_{m \geq 1} z^m P(m,t) = 0.1
\]

\[
0.2
\]

\[
0.3
\]

\[
0.4
\]

\[
0.6
\]

\[
0.8
\]

\[
0.9
\]

\[ (a) \]

\[
C(x) \]

\[
\xi(\rho)
\]

\[ (b) \]

\[
P(m)
\]

\[
P(m')
\]

Figure 4: (a) Particle cluster distribution \( C(x) \) as a function of cluster size \( x \) for different densities follow Poisson distribution. Inset shows exponential growth of correlation length as a function of density. (b) The stationary-state gap distribution \( P(m) \) shows peaks at multiples of four gap sizes for various densities. Inset shows the exponential decay of the distribution of the peaks \( P(m') \) for all densities. The rates of attachment and detachment here are \( P_{on} = S_{off} = 0.8 \), \( P_{off} = S_{on} = 0.2 \).
of the master equation in the stationary state. The detailed calculation and comparison of results with Monte Carlo simulations for maximum step size $m_s = 2$ are presented in Appendix A. For any arbitrary jump size, the steady-state gap distribution has a polynomial solution and takes the following form for rate Eq. [\ref{eq:unl}] \cite{18}

$$P(m) = \sum_{i=1}^{m_s} \alpha_i q_i^m .$$  

(7)

We can also define the current in terms of the gap distribution as

$$j(\rho) = \rho \sum_{k=1}^{m_s} P(k) \sum_{n=1}^{k} u_n(k) .$$  

(8)

Further, it is interesting to determine the dynamical behavior of the system in the stationary state. Earlier studies have shown that the variants of TASEP in one dimension fall in KPZ universality class, where dynamic exponent $z = 3/2$ \cite{19, 20}. We calculate the stationary state mean square displacement of tagged particles defined as $\langle \delta \sigma^2(t) \rangle = \langle d^2 \rangle - \langle d \rangle^2$, where $d$ is the average displacement traveled by the tagged particle and the angular bracket is an average over the different realizations starting from the same initial conditions for this N-motors system. Our simulation results show the same characteristic features as observed in the case of 1D TASEP \cite{19}. We see the initial KPZ growth with an exponent $2/3$ which is a signature of the TASEP universality class, followed by diffusion. The standard finite size scaling form shows perfect scaling collapse with dynamical exponent $z_s = 3/2$, as shown in Fig. 5(a).

3.1.2. Transient behavior: Next, we investigate the dynamics of the system starting from random initial configurations and calculate the mean square displacement of the motors in time,

$$\langle \delta r^2(t) \rangle = \langle r^2 \rangle - \langle r \rangle^2 ,$$  

(9)

where $r(t) = \frac{1}{N} \sum_{i=1}^{N} x(t)$ is the average displacement of the motors over the entire lattice and the angular bracket represents ensemble averaging.

We measure the mean square displacement for various densities as well as for different attachment and detachment rates. They all display power law behavior with time $\langle \delta r^2(t) \rangle \sim t^\gamma$ as shown in Fig. 3(b). After a small initial time window $t_{mic} \sim 100$ time steps, the intermediate time growth of mean square displacement shows anomalous diffusion, which means faster than diffusive behavior. The best fit of the transient regime gives growth exponent $\gamma \approx 1.3 \pm 0.1$ before it crosses over to a standard diffusive regime at later times where $\gamma$ is one. We also observe that the crossover time depends on the density of the motors present in the system. This kind of super-diffusive behavior has been observed experimentally in the dynamical regime of molecular motors and other active cellular matter \cite{21, 22, 23}. In most biological systems, short-range fluctuations are responsible for the diffusive propagation, whereas long-range fluctuations arising from directed transport driven by chemical energy cause super-diffusive dynamics \cite{24, 25}. One can interpret the crossover from super-diffusive to diffusive behavior in our simulations with a similar argument. At early times, the motion is primarily dictated by individual hops resulting from ATP hydrolysis and uncorrelated collective dynamics. This weak super-diffusive power law could perhaps also be attributed to logarithmic correction. After the transient period, the dominant stochastic collisions
between the particles slow down the growth of mean square displacement, which results in standard diffusive behavior in the long-time regime. We also evaluate the dynamic scaling exponent using the finite-size scaling relation,
\[ \langle \delta r^2(t) \rangle \propto L^{\xi} f \left( \frac{t}{L^z} \right). \] (10)

The best data collapse gives the exponents \( \xi = 1 \) and \( z = 3/2 \), as shown in the inset of Fig. 5(b).

3.2. Open Boundary Conditions

In this section, we discuss the results and analysis of the collective behavior of an N-motor system with open boundary conditions. The open boundary lattice is a more realistic depiction of the biological system as microtubules are open-ended tracks on which a motor can enter and exit from the left end (head) and the right end (tail), respectively. A motor enters with probability \( \alpha \) provided that the first site is empty and exits from last lattice site with probability \( \beta \). The rules of hopping in bulk are the same as in the periodic boundary case. However, if the particle reaches the last lattice site while hopping with the ATP dependent jump probability, then it exits the lattice. We perform simulations with three different rates of influx and escape: \( \alpha = 2\beta \), \( \alpha = \beta \), and \( \alpha = \beta/2 \), starting with different initial densities. For arbitrary \( m_s \), one can write the per-site occupancy dynamics as

\[ \frac{d\rho_1}{dt} = \alpha(1 - \rho_1) - v_s \rho_1 (1 - \rho_2), \]
\[ \frac{d\rho_k}{dt} = \left[ v_j \rho_{k-1} + \bar{v} \rho_k (1 - \rho_{k-1}) \Theta(k-2) \right] (1 - \rho_k) \rho_{k+1} + \sum_{j=1}^{\min(k-1,m_s)} v_j \rho_{k-j} \prod_{i=0}^{j-1} (1 - \rho_{k-i}) - v_s \rho_k (1 - \rho_{k+1}), \quad 1 < k < L \]
\[
\frac{d \rho_L}{dt} = \sum_{j=1}^{m_s} v_j \rho_{L-j} \prod_{i=0}^{j-1} (1 - \rho_{L-i}) - \beta \rho_L ,
\]
(13)
where \( v_s = \sum_{j=1}^{m_s} v_j, \bar{v} = v_2 + v_3 + v_4, \tilde{v} = v_3 + v_4, \) and \( \alpha, \beta \) are the entry and exit rates, respectively.

### 3.2.1. Steady state properties:
We first analyze the stationary state density profile over the lattice. Interestingly, as can be seen in Fig. 6, we observe oscillatory behavior near the boundary, where the particles enter the system. The average density peaks at those lattice sites which are multiples of the maximum jump size \( m_s \), with the amplitude of the peaks decaying exponentially as one moves further into the bulk. The characteristic decay length depends on the influx rate; the larger \( \alpha \), the faster the decay. The depth of these oscillations into the bulk of the system also decreases with the increasing influx rates, see Fig. 6(a). Significantly high influx rate causes crowding near the entry site forcing the motors to take smaller steps. The depth of oscillations into the bulk also decreases upon lowering \( P_{on} \), as shown in Fig. 6(b). Reducing \( P_{on} \) implies an increase in the attachment rate \( S_{on} \) of secondary ATP binding sites, which consequently increases the probability of taking smaller step sizes. Thus the amplitude of these oscillations decays and vanishes faster displaying a TASEP-like tangent profile [26]. From our simulation results, we conclude that the mean density in bulk never exceeds \( \rho = 0 \), even for significantly high influx rates. For large \( P_{on} \) and small \( S_{on} \) values, the bulk density profile is almost flat. The gap distribution shows similar peaks at multiples of the maximum step-size with exponentially decaying amplitude as discussed for case of periodic boundary conditions, see Fig. 7(a).

### 3.2.2. Transient behavior:
To understand the dynamics of the system, we furthermore analyze the mean square displacement \( \langle \delta r^2(t) \rangle \) during transient regime, as was done for periodic boundary conditions in sec. 3.1. During the growth of the mean square displacement, we observe three
Figure 7: (a) The stationary state gap distribution $P(m)$ shows peaks at multiples of 4 for different rates $\alpha$ and $\beta$, and the inset shows the exponential decay of these peaks with gap size $m$. (b) Growth of fluctuations for different starting densities, for the case $\alpha = 2\beta = 2/3$. The inset shows the finite size scaling collapse of mean square displacement with the dynamical exponent, $z = 1$.

different growth regimes; initial time dynamic exhibits a combination of super-diffusive and ballistic growth ($\langle \delta r^2(t) \rangle \sim \Gamma t^{1.2} + \Gamma' t^2$, where $\Gamma$ and $\Gamma'$ are fitting parameters) followed by complete ballistic growth ($\langle \delta r^2(t) \rangle \sim t^2$) in the intermediate regime. The long-time behavior of the system is predominantly diffusive. This ballistic growth preceding the diffusive stationary state can be explained by the accelerated motion of the particles in the intermediate regime as there is enough empty space present in front of them. We also probe the effect of different starting densities on the growth of fluctuations. As shown in Fig. 7(b), for zero initial density one observes a more prolonged ballistic regime; with the increase in initial density, the pure ballistic regime becomes negligible. For finite initial density, we observe prolonged mixed ballistic and diffusive dynamics. However, in the long-time regime, the dynamics is independent of the initial densities, and the effect of stochastic forces start to become evident, forcing the motors to undergo diffusion [27, 28]. Furthermore, plots for different system sizes collapse according to the finite-size scaling relation (10) with exponents $\xi = 1$ and $z = 1$, as shown in the inset of Fig. 7(b)). The dynamical exponent $z = 1$ is the resultant of ballistic growth of fluctuations.

4. Conclusion and Outlook

Our stochastic modeling of dynein motor transport on a lattice with the incorporation of varying hop sizes manifested many exciting results. The study of the stationary state current shows a breakdown of particle-hole symmetry depending on the choice of attachment and detachment rates. The very intuitive features of the gap distribution allowed us to obtain a better insight into the collective behavior and self-organizing nature of the dyneins for both open and periodic boundary conditions. The gap distribution peaks at lattice sites which are multiples of the maximum step size, signifying that the motors organize themselves so they can take the maximum jumps possible. We also carried out the a mean-field calculation for the gap distribution. For the more realistic scenario of open boundary conditions, our simulations capture a damped oscillating behavior of the
density profile. The decay length highly depends on the attachment and detachment probabilities, as well as the influx and escape rates of the motors. Similar oscillations, albeit undamped unlike in our model, have been observed in earlier studies of dynein motors using cellular automata; here, we would like to emphasize the fact that different modeling approaches lead to very different results. The cause of this difference is still an open question. For the mean square displacement, we observe two regimes, an early time of fast growth followed by diffusive growth as the system approaches the stationary state. In the initial transient period, open and periodic boundary conditions show ballistic and superdiffusive growth with exponents 2 and 1.3, respectively. Future works may involve adapting this model further to include other aspects of biological systems such as controlling the ATP concentration; non-conserved bulk dynamics by incorporating the evaporation of particles, etc. These possibilities of modifications may render the model more realistic, and we would like to pursue these issues in the future.

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Appendix A.

We analytically solve for the gap distribution $P(m)$ for the case when a motor can hop to maximally 2 empty sites in front of it. The rate of hopping $n$ steps with $m$ empty spaces in front of the motor is,

$$\alpha_m(n) = v_1 \delta_{n,1} \delta_{m,1} + \theta(m-2)(v_2 \delta_{n,1} + v_3 \delta_{n,2}) . \quad (A.1)$$

The master equations for the time dependent gap distribution $P(m,t)$ are,

$$\frac{dP(0,t)}{dt} = -P(0,t) \left[ v_1 P(1,t) + (v_2 + v_3) \sum_{m=2}^{\infty} P(m,t) \right]$$

$$+ v_1 P(1,t) + v_3 P(2,t) , \quad (A.2)$$

$$\frac{dP(1,t)}{dt} = -P(1,t) \left[ v_1 (1 + P(1,t)) + (v_2 + v_3) \sum_{m=2}^{\infty} P(m,t) \right]$$

$$+ v_3 P(3,t) + v_1 P(1,t) P(0,t) + v_2 \sum_{m=2}^{\infty} P(m,t)P(0,t) , \quad (A.3)$$

$$\frac{dP(m,t)}{dt} = -P(m,t)(v_2 + v_3) - P(m,t) \left[ v_1 P(1,t) + (v_2 + v_3) \sum_{m=2}^{\infty} P(m,t) \right]$$

$$+ v_2 P(m+1,t) + v_3 P(m+2,t) + P(m-1,t)v_1 P(1,t)$$

$$+ v_2 \sum_{m=2}^{\infty} P(m,t) + v_3 P(m-2) \sum_{m=2}^{\infty} P(m,t) . \quad (A.4)$$
Since the total probability is conserved, \( \sum_{m=0}^{\infty} P(m, t) = 1 \), defining \( \sum_{m=k}^{\infty} P(m, t) = S_k \) and using the conservation law \( P(0, t) + \sum_{m=1}^{\infty} P(m, t) = 1 \), we have
\[
P(0, t) = 1 - S_1.
\] (A.5)

Similarly, \( P(1, t) \) can be represented as \( S_1 - S_2 \). Using these substitutions, we arrive at the simplified form of the evolution equation,
\[
\frac{dP(0, t)}{dt} = -P(0, t)\left[v_1 P(1, t) + (v_2 + v_3)S_2 \right] + v_1 P(1, t) + v_3 P(2, t),
\] (A.6)
\[
\frac{dP(1, t)}{dt} = -P(1, t)\left[v_1 (1 + S_1 - S_2) + (v_2 + v_3)S_2 \right] + v_2 P(2, t) + v_3 P(3, t) + \left[ v_1 (S_1 - S_2) + v_2 S_2 \right] P(0, t),
\] (A.7)
\[
\frac{dP(m, t)}{dt} = -P(m, t)\left[(v_2 + v_3)(1 + S_2) + v_1 (S_1 - S_2) \right] + v_2 P(m + 1, t) + v_3 P(m + 2, t) + v_3 S_2 P(m - 2, t) + P(m - 1)[v_1 (S_1 - S_2) + v_2 S_2] \quad m \geq 2.
\] (A.8)

Defining the generating function, \( G = \sum_{m=1}^{\infty} z^m P(m, t) \), we can write the evolution equation as,
\[
\frac{dG}{dt} = \frac{d}{dt} \sum_{m=1}^{\infty} z^m P(m, t) = \left[(1 + S_2)(v_2 + v_3) + v_1 (S_1 - S_2) \right] + w_2 z^{-1} + w_3 z^{-2} + [v_1 (S_1 - S_2) + w_2 S_2]z
\]
\[
+ w_2 S_2 z^2 \right] G + z(v_2 + v_3 - v_1)P(1, t) + v_2 P(1, t) - w_3 z^{-1} P(1, t)
\]
\[
- v_3 P(2, t) + [v_1 (S_1 - S_2) + w_2 S_2]z P(0, t).
\] (A.9)

In the stationary state, the probabilities are time independent. Hence, setting \( \frac{dP(0, t)}{dt} = 0 \) equal to zero, one can obtain,
\[
v_3 P(2) = -v_1 P(1) + P(m)[v_1 P(1) + (v_2 + v_3)S_2].
\] (A.10)

To solve for stationary state, we set \( \frac{dG}{dt} = 0 \), and plug Eq. \( \text{A.10} \) in Eq. \( \text{A.9} \) which gives us the following polynomial equation,
\[
\left[-z^4 v_3 S_2 - z^2 [v_1 (S_1 - S_2) + v_2 S_2] + z^2 [(1 + S_2)(v_2 + v_3) + v_1 (S_1 - S_2)] \right]
\]
\[- v_2 z - v_3 \right] G = z^4 v_3 S_2 (1 - S_1) + z^2 \left[(v_2 + v_3 - v_1 S_1)(S_1 - S_2) v_2 S_2 (1 - S_2) \right]
\]
\[- z^2 \left[v_1 (S_1 - S_2) + (v_2 + v_3)S_2 (1 - S_1) + (v_1 - v_2)(S_1 - S_2) - v_3 (S_1 - S_2) \right] z.
\] (A.11)

Simplifying the above equation by taking out the common factor of \( (z - 1) \), we get
\[
\left[-z^3 v_3 S_2 - z^2 [(v_2 + v_3)S_2 + v_1 (S_1 - S_2)] + z(v_2 + v_3) + v_3 \right] G =
\]
\[z^3 v_3 S_2 (1 - S_1) + z^2 [(v_2 + v_3)S_1 (1 - S_2) - v_1 S_1 (S_1 - S_2)] + zv_3 (S_1 - S_2).
\] (A.12)
Further, we expand $G$, equate all coefficients for $z^m$ from both sides of (A.12), and obtain the recursion relation for $P(m)$ which is also calculated in [18]. In case of $m_s = 2$, the recurrence relation for $P(m)$ is given as

$$P(m)v_3 + P(m-1)(v_2 + v_3) - P(m-2)(S_1v_1 - S_2(v_2 + v_3 - v_1)) - P(m-3)S_2v_3 = 0.$$  \hspace{0.5cm} (A.13)

Assuming a polynomial solution, $P(m) x^m$ and using in (A.13), we get a third order polynomial in $x$,

$$v_3x^3 + (v_2 + v_3)x^2 - (S_2(v_2 + v_3 - v_1) + S_1v_1)x - S_2v_3 = 0.$$  \hspace{0.5cm} (A.14)

Solution of above equation has three roots $x_1, x_2, x_3$ and hence $P(m) = c_1x_1^m + c_2x_2^m + c_3x_3^m$. Using conservation laws Eq.6 we consider that the coefficients $c_3 = 0$ and $c_1, c_2$ values depend on the rates. We solve two consecutive equations for specifying the values of the transition rates, $v_1, v_2, v_3$ and the density the $\rho$ and solved for all the unknowns. We have shown the comparison of the solution with Monte-Carlo simulation of $N$-motor system in Fig. A1, $v_i$ depends on the attachment and detachment rates as,

$$v_2 = P_{on}(1 - P_{off})(S_{on}(1 - S_{off})),$$
$$v_3 = P_{on}(1 - P_{off})(1 - S_{on}) + S_{on}S_{off},$$
$$v_1 = v_3\rho + v_2.$$ \hspace{0.5cm} (A.15)

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