Interacting motile agents: Taking a mean-field approach beyond monomers and nearest-neighbor steps

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We consider a discrete agent-based model on a one-dimensional lattice, where each agent occupies L sites and attempts movements over a distance of d lattice sites. Agents obey a strict simple exclusion rule. A discrete-time master equation is derived using a mean-field approximation and careful probability arguments. In the continuum limit, nonlinear diffusion equations that describe the average agent occupancy are obtained. Averaged discrete simulation data are generated and shown to compare very well with the solution to the derived nonlinear diffusion equations. This framework allows us to approach a lattice-free result using all the advantages of lattice methods. Since different cell types have different shapes and speeds of movement, this work offers insight into population-level behavior of collective cellular motion.

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I. INTRODUCTION

It is important to understand biological or physical processes on two levels: the local behavior of individuals and the global properties of the group as a whole. Methods for converting stochastic agent-based models of local behavior into partial differential equation (PDE) descriptions for the agent occupancy as a continuous function have therefore been studied fairly extensively [1–5]. Many of these models, however, study spherical agents attempting to move their own diameter each time step. In a biological context, cells or micro-organisms being modeled can vary enormously in their shape and movement. Some work exists on models of agents of larger sizes, although these models mostly restrict movement to the neighboring sites on a lattice [6,7], which means that the agents can only move distances smaller than their length. In this paper we construct two agent-based models which remove these conditions. We allow agents to be any length and to move any distance (cf. Dyson *et al*. [8]).

There are two types of agent-based models: lattice-based models, where agents move between sites of a lattice; and lattice-free models, where agents move freely without a lattice structure [9,10]. Most biological or physical processes being modeled do not have an intrinsic lattice structure, making a lattice-free model more realistic in many cases, while lattice-based models often have the advantages of easier calculations. However, the differences between the simulation results of the two model types are frequently small. We use a lattice model, but without limiting the size of the agents or the distance moved each time step to only one lattice spacing. By freeing the choice of agent length and movement distance to any integer multiple of the lattice spacing, we can achieve a model with any required rational relationship between them. If we keep this relationship constant while increasing the agent length and movement distance simultaneously, we move towards a lattice-free model, while keeping the advantages of a lattice-based model.

The standard methodology for a mean-field treatment of monomer agents (i.e., agents that occupy only one site of the lattice) moving only to their nearest-neighbor sites is accurate compared to simulations for a broad range of models [11–14]. Different mean-field methodologies for extended agents have emerged, producing different PDE descriptions [6,7]. In a previous paper [15], we showed that careful arguments based on the use of indicator variables are helpful in finding better mean-field approximations for dimers than those based on the crudest local independence assumptions. We adopt a similar basic strategy here.

We discuss two models of agent movement over more than one lattice spacing each time step. Although the basic ideas that we explain here can be implemented on any periodic lattice, we confine our discussion to one dimension. In both models, each lattice site can be occupied by, at most, one agent, defining a simple exclusion process. In the first model (discussed in Secs. II and III) we consider agents that may only move a fixed integer, distance d sites on the lattice; if there is another agent occupying any site from its current position up to and including its destination, then the move is aborted. In the second model (discussed in Sec. IV), agents that are prevented from moving the full distance d sites by the presence of another agent can instead move as far as possible; that is, the agent moves to the site adjacent to the agent preventing the full-distance move.

We verify our results for both models by comparing the PDE solutions to the simulation data on agents moving according to the model rules, averaged over many realizations.

II. MONOMER AGENTS WITH A FIXED MOVEMENT DISTANCE

We begin by considering agents occupying a single site, each moving randomly on a one-dimensional lattice, with the restriction that each lattice site may be occupied by, at most, one agent. We allow agents to move by hopping a fixed distance to the left or to the right, though agents may only move if all of the sites that they are attempting to move through, including their final destination, are empty.

A. Probabilistic model

We consider a one-dimensional lattice with bonds of length Δ, with a generic site x, and we write $i = \Delta^{-1}x$, with $i \in \mathbb{Z}$. There are N agents (each occupying a single site) on the lattice,

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FIG. 1. (Color online) Monomer agents: If $d = 1$, the center [open (green) circle] agent can move in either direction. If $d = 2$ the center [open (green) circle] agent can move right but cannot move left, as the left [open (red) circle] agent is occupying the site. If $d \geq 3$, the center [open (green) circle] agent cannot move in either direction because there is an agent preventing the move in both directions.

which attempt to move exactly d lattice sites in either direction without bias; if another agent occupies any of the d sites the agent is attempting to move through, the move is aborted. Figure 1 illustrates allowed and blocked movements for agents with different distances of movement d.

At each time step, we choose an agent randomly and suppose that the agent will attempt to move with probability P. The probability that any given agent is selected is $1/N$ as each agent is chosen with equal probability. (We note that this is an alternate but equivalent method to the one frequently used. In other work [1,5–7,14,15], there are N independent sequential random choices of agent at each time step of length τ.) We consider the indicator variable

$$\gamma_n(i) = \begin{cases} 1 & \text{if site } i \text{ is occupied by an agent after } n \text{ time steps,} \\ 0 & \text{otherwise.} \end{cases}$$

We can therefore calculate the change in probability of occupancy of site i from time step n to time step $n+1$. There are four ways that a single agent move can change the occupancy of site i, reflected in the four terms on the right-hand side of Eq. (1) below, respectively: an agent already at i moves left to vacate it; an agent already at i moves right to vacate it; site i is empty and there is an agent at site $i+d$ which moves to the left; or site i is empty and there is an agent at site $i-d$ which moves to the right [16]. We have

$$\begin{aligned} \mathbb{P}(\gamma_{n+1}(i)=1) - \mathbb{P}(\gamma_n(i)=1) = &-\frac{P}{2N}\mathbb{P}(\gamma_n(i)=1,\gamma_n(i-s)=0 \quad \text{for} \quad 1 \leq s \leq d) \\ &-\frac{P}{2N}\mathbb{P}(\gamma_n(i)=1,\gamma_n(i+s)=0 \quad \text{for} \quad 1 \leq s \leq d) \\ &+\frac{P}{2N}\mathbb{P}(\gamma_n(i+d)=1,\gamma_n(i+s)=0 \quad \text{for} \quad 0 \leq s \leq d-1) \\ &+\frac{P}{2N}\mathbb{P}(\gamma_n(i-d)=1,\gamma_n(i-s)=0 \quad \text{for} \quad 0 \leq s \leq d-1). \end{aligned} \tag{1}$$

In order to use a mean-field approach, we require probabilities of occupancies of single sites and so we must make an approximation of independence of occupancy of neighboring sites. For example, the first compound event probability in Eq. (1) can be approximated as

$$\begin{aligned} &\mathbb{P}(\gamma_n(i)=1,\gamma_n(i+s)=0 \quad \text{for} \quad 1 \leq s \leq d) \\ &\quad = \mathbb{P}(\gamma_n(i)=1)\mathbb{P}(\gamma_n(i+s)=0 \quad \text{for} \quad 1 \leq s \leq d) \\ &\quad = \mathbb{P}(\gamma_n(i)=1)\prod_{s=1}^{d}[1-\mathbb{P}(\gamma_n(i+s)=1)], \end{aligned} \tag{2}$$

and we make similar approximations to simplify the remaining terms in Eq. (1).

To simplify the notation, we write

$$r_n(i) = \langle \gamma_n(i) \rangle = \mathbb{P}(\gamma_n(i)=1). \tag{3}$$

Using the approximation of independence just described, Eq. (1) can be written as a discrete-time master equation:

$$\begin{aligned} &r_{n+1}(i) - r_n(i) \\ &\quad = \frac{P}{2N}\left\{[r_n(i+d)-r_n(i)]\prod_{s=1}^{d-1}[1-r_n(i+s)]\right. \\ &\qquad \left. +[r_n(i-d)-r_n(i)]\prod_{s=1}^{d-1}[1-r_n(i-s)]\right\}. \end{aligned} \tag{4}$$

B. Continuum limit

We take the appropriate continuum limit as the distance Δ and the time τ/N between consecutive time steps tend to 0 to obtain a PDE description for the average occupancy. We use the time step τ/N so that, on average, each agent will be chosen to move once during the time τ. We return to $x = \Delta i$, define the time $t = n\tau/N$, and write $r_n(i) = C(x,t)$, where $C(x,t)$ is a continuous variable representing the local average occupancy. Supposing C to be sufficiently smooth, we use a Taylor expansion,

$$r_n(i+k) = C + k\Delta\frac{\partial C}{\partial x} + \frac{(k\Delta)^2}{2}\frac{\partial^2 C}{\partial x^2} + o(\Delta^2), \tag{5}$$

where C and its spatial derivatives are evaluated at (x,t). Equation (4) can therefore be rewritten as

$$\begin{aligned} \frac{\tau}{N}\frac{\partial C}{\partial t} + o(\tau) = \frac{P}{2N}(d\Delta)^2(1-C)^{d-2}\left[(1-C)\frac{\partial^2 C}{\partial x^2}\right. \\ \left. -(d-1)\left(\frac{\partial C}{\partial x}\right)^2\right] + o(\Delta^2). \end{aligned} \tag{6}$$

Taking the limit $\Delta, \tau \to 0$ simultaneously while keeping the ratio Δ^2/τ constant gives us the nonlinear differential equation

$$\frac{\partial C}{\partial t} = D_0\frac{\partial}{\partial x}\left(\mathcal{D}(C)\frac{\partial C}{\partial x}\right), \tag{7}$$

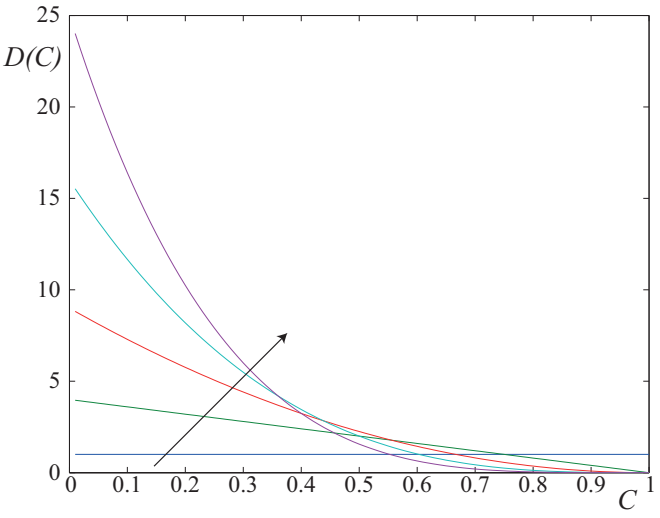

FIG. 2. (Color online) Diffusion coefficient for monomers ($L = 1$), $\mathcal{D}(C) = d^2(1-C)^{d-1}$, with movement distance $d = 1, 2, 3, 4, 5$ [Eq. (7)]. The arrow indicates increasing d.

where

$$\mathcal{D}(C) = d^2(1-C)^{d-1} \tag{8}$$

and

$$D_0 = \frac{P}{2} \lim_{\Delta,\tau\to 0} \frac{\Delta^2}{\tau}. \tag{9}$$

We note that when $d = 1$ and agents can only move to their nearest-neighbor sites, with the simple exclusion constraint, then Eq. (7) reduces to linear diffusion as expected [5,11,14,17].

The diffusion coefficient $\mathcal{D}(C)$ in Eq. (8) is a polynomial in C, in common with many other models [5,12,14], and D_0 is the usual expression in one dimension. The degree of the polynomial depends on the movement distance d. As shown in Fig. 2, for lower values of the density the diffusion coefficient increases as the distance d increases, while the opposite occurs for higher densities. This is the behavior we might have expected: at low densities the agents are unlikely to find their movement blocked by another agent and so are able to move farther, but at higher densities the greater distance that needs to be empty reduces the chances that an agent will be able to move. Note that the diffusivity at maximum density, $\mathcal{D}(1)$, is 0 for values of $d > 1$. As noted above, this does not occur when $d = 1$, where $\mathcal{D}(C) = 1$ independent of C. Further comments on the behavior of the diffusivity and its relationship to the flux of agents are left to Sec. V.

The d^2 in the coefficient of $\mathcal{D}(C)$ occurs because the movement is unbiased and therefore the first nonzero term is $O(\Delta^2)$, and the distance of movement is d multiples of the lattice spacing Δ.

C. Simulations

Simulation results were produced in MATLAB on a lattice with $1 \le x \le 200\,d$ and agents initially placed in the center of the lattice at half the maximum density (see Appendix for more details). The results were averaged over 50 000 simulations to provide the results shown in Fig. 3. These results are compared to solutions to the nonlinear diffusion equation [Eqs (7) and (8)]. We observe that agents spread out with time and that the PDE solutions give an excellent fit to the simulation data, when $d = 2$ and $d = 3$. In general the fit is good for modest values of d, but deteriorates gradually as d is increased.

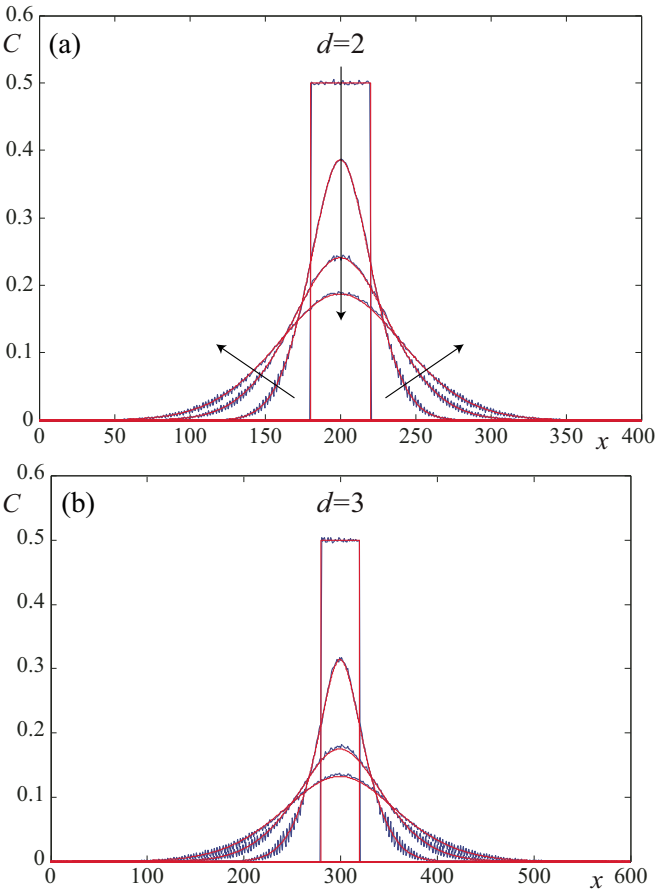

FIG. 3. (Color online) Monomer agents moving d lattice sites: Solutions to Eq. (7) [medium-gray (red) curve] compared to the average of 50 000 simulations [dark-gray (blue) curve] at times $t = 100$, 300, and 500. (a) $d = 2$. The initial condition (shown) has agents between $181 \leqslant x \leqslant 220$. (b) $d = 3$. The initial condition (shown) has agents between $281 \leqslant x \leqslant 320$. Note the different scales on the x axes: for larger values of d the outermost agents move farther, and so a larger region is needed to prevent interference with the boundaries for $t \leqslant 500$. Equation (7) was solved using MATLAB **pdepe** with $\delta x = 0.1$. Arrows in (a) indicate increasing time.

The averaged simulation data shown in Fig. 3 have oscillations away from the center of the profiles. Such oscillations do not occur if monomers move only to nearest-neighbor sites, that is, when $d = 1$. In contrast, the regular oscillations seen are always observed and do not decrease as the number of simulations averaged increases. They have a periodicity equal to the distance moved d and reflect a slight difference in the probabilities of the sites being occupied. We discuss this first for the specific case $d = 2$, in which the agents are initially placed between $x = 181$ and $x = 220$ inclusive. While the agents are initially placed randomly, the leftmost agent is more likely to be initially placed on an odd-numbered site, and similarly, the agents that reach farther left are more likely

to have started at an odd-numbered site and less likely to have started at an even-numbered site. As agents can move exactly two sites or not at all, this means that agents that start on odd sites stay on odd sites and therefore odd sites to the left are more likely to be occupied than even sites to the left. The same argument explains the peaks on even sites on the other side of the simulation, and if we consider sites with $x \equiv n \mod d$ rather than odd/even sites, then the same argument explains the periodicity of results for other values of d. Although the difference in probability is small, it is consistent for all simulations and therefore seen in the results, but not in the solution to Eq. (7). For example, when $d = 2$, if half of the simulations have an initial region shifted by one lattice spacing, the oscillations disappear.

III. INTEGER LENGTH AGENTS WITH A FIXED MOVEMENT DISTANCE

We now extend the model to allow the agents to occupy more than one site of the one-dimensional lattice. Each agent now has a length $L\Delta$ for some positive integer L and moves a distance $d\Delta$ along the lattice. This allows the agents, with appropriate choices of L and d, to move any fraction of their length and reduces one of the restrictions imposed by the lattice. As the case $L = 1$ has been covered in Sec. II, for the present we assume that $L \geq 2$. However, the final results obtained here when setting $L = 1$ are consistent with those obtained in Sec. II [Eq. (7)].

A. Probabilistic model

As in Sec. II, we consider a one-dimensional lattice with bonds of length Δ, a generic site x with $i = \Delta^{-1}x \in \mathbb{Z}$, and N agents on the lattice, which attempt to move exactly d lattice sites without directional bias and cannot overlap. At each time step we choose an agent randomly with equal probability and suppose that the agent will attempt to move with probability P.

As each agent can occupy more than one site, the site occupancy of the *rightmost end* of the agent will be determined using indicator variables as by Penington *et al.* [15]. We use the indicator variable

$$\gamma_n(i) = \begin{cases} 1 & \text{if site } i \text{ is occupied by the rightmost end of an agent after } n \text{ time steps,} \\ 0 & \text{otherwise.} \end{cases}$$

We can calculate the change in the probability of occupancy of site i by the rightmost end of an agent from time step n to time step $n + 1$. Because agents cannot overlap, we know that if there is the rightmost end of an agent at some site j, then there cannot be the rightmost end of another agent at site $j + s$ for any s with $-L < s < L$, and equivalently, this region must be empty for an agent to move to site j. Since $\gamma_n(j) = 1$ implies that $\gamma_n(j + s) = 0$ for $-L < s < L$, we do not write this explicitly, to simplify the notation.

As in Sec. II, there are four ways that a single agent move can change the occupancy of site i: an agent already at i moves left to vacate it; an agent already at i moves right to vacate it; site i is empty and there is an agent at site $i + d$ which moves to the left; or site i is empty and there is an agent at site $i - d$ which moves to the right. The change in the probability that site i is occupied by the rightmost end of an agent at time step $n + 1$ is therefore given by

$$\begin{aligned} \mathbb{P}(\gamma_{n+1}(i) = 1) - \mathbb{P}(\gamma_n(i) = 1) = &-\frac{P}{2N}\mathbb{P}(\gamma_n(i) = 1,\ \gamma_n(i - s) = 0 \quad \text{for} \quad L \leq s \leq d + L - 1) \\ &- \frac{P}{2N}\mathbb{P}(\gamma_n(i) = 1,\ \gamma_n(i + s) = 0 \quad \text{for} \quad L \leq s \leq d + L - 1) \\ &+ \frac{P}{2N}\mathbb{P}(\gamma_n(i + d) = 1,\ \gamma_n(i + s) = 0 \quad \text{for} \quad 1 - L \leq s \leq d - L) \\ &+ \frac{P}{2N}\mathbb{P}(\gamma_n(i - d) = 1,\ \gamma_n(i - s) = 0 \quad \text{for} \quad 1 - L \leq s \leq d - L). \end{aligned} \tag{10}$$

In order to use a mean-field approach, we require the probabilities of occupancies of single sites and so we must make an approximation. At this point in Sec. II we approximated the probability of consecutive sites being empty with the product of those probabilities. For agents with length $L > 1$, this is not a good approximation to make, because we know that $\mathbb{P}(\gamma_n(j) = 1,\ \gamma_n(j + 1) = 1) = 0$ since two agents cannot overlap.

When $L = 1$ there were only two possible states for a lattice site: either it was occupied by an agent, and therefore $\gamma_n(j) = 1$, or it was empty and available for any agent to move into. Now we have a third possibility: for every occupied position there are $L - 1$ other lattice sites with $\gamma_n(j) = 0$ that are occupied by an unlabeled part of an agent.

Our first approximation is that the probability that a position is occupied, $\mathbb{P}(\gamma_n(j) = 1)$, varies slowly in j over a length scale of an agent. Under this approximation, and in the absence of any knowledge of the occupancy of neighboring positions, we suppose that a lattice site is equally likely to be occupied by the rightmost end of an agent as any other part. So if

$$\mathbb{P}(\text{site } j \text{ occupied by rightmost end of an agent}) = \mathbb{P}(\gamma_n(j) = 1,$$

which is our definition of $\gamma_n(j)$, then

$$\mathbb{P}(\text{site } j \text{ occupied by leftmost end of an agent}) \approx \mathbb{P}(\gamma_n(j) = 1),$$

and the same approximation is made for any other part of an agent. Obviously this is not entirely accurate: if the leftmost end of an agent is at site j, then its rightmost end will be at site $(j + L - 1)$ and $\mathbb{P}(\gamma_n(j + L - 1) = 1)$ may not be the same as $\mathbb{P}(\gamma_n(j) = 1)$. But as we see in the simulations, even when the initial condition is a step function this approximation still produces good results.

Using this approximation, we now return to the three possible states for any lattice site j. The three states cannot occur simultaneously (if a site is completely vacant, it cannot also be occupied by the rightmost end of an agent, for example) so the probabilities must sum to unity. So

$$\mathbb{P}(\text{site } j \text{ occupied by rightmost end of an agent}) = \mathbb{P}(\gamma_n(j) = 1),$$

$$\mathbb{P}(\text{site } j \text{ occupied by an unlabeled part of an agent}) \approx (L-1)\mathbb{P}(\gamma_n(j) = 1),$$

$$\mathbb{P}(\text{site } j \text{ completely vacant of any agent}) \approx 1 - L\mathbb{P}(\gamma_n(j) = 1).$$

If site j is occupied by an unlabeled part of an agent, then there are $(L-1)$ different possible parts, and we approximate the probability that site j is occupied by any one unlabeled part of an agent with $\mathbb{P}(\gamma_n(j) = 1)$. For agents with $L > 2$ the different possibilities also cannot occur simultaneously (as the site cannot be occupied by both the leftmost end of an agent and the center of an agent, for example) and so the probability that any one of them occurs is therefore their sum.

Now suppose we know that there is another agent to the right of lattice site j: $\gamma_n(j+L) = 1$. Site j could still be occupied by the right-hand end of a new agent or it could be empty, but we know that it *cannot* be occupied by an unlabeled part of an agent, for then the two agents would overlap. We therefore make our second approximation: the relative probabilities of the two possible states remain the same. Symbolically,

$$\mathbb{P}(\gamma_n(j) = 1 \,|\, \gamma_n(j+L) = 1) \approx \frac{\mathbb{P}(\gamma_n(j) = 1)}{1 - (L-1)\mathbb{P}(\gamma_n(j) = 1)}. \tag{11}$$

In words, the probability that site j is occupied by the rightmost end of an agent, when there is an agent with its leftmost end at site $(j+1)$, is the probability that site j is occupied by the rightmost end of an agent divided by the probability that site j is not occupied by an unlabeled part of an agent (since that would be impossible). This is effectively stating that the probability that two agents are in adjacent positions is higher than it would be if the two events were independent. This can be clearly seen in an alternative form of Eq. (11):

$$\mathbb{P}(\gamma_n(j) = 1,\, \gamma_n(j+L) = 1) \approx \frac{\mathbb{P}(\gamma_n(j) = 1)\mathbb{P}(\gamma_n(j+L) = 1)}{1 - (L-1)\mathbb{P}(\gamma_n(j) = 1)}. \tag{12}$$

We note that if $L = 1$, this reduces to the approximation of independence of the occupancies of adjacent sites for monomer agents. We discuss the agreement between simulations and solutions of PDEs derived from using Eq. (11) and similar approximations presently. We tested the accuracy of approximation (11) directly by simulation of an equilibrated finite system for a range of agent concentrations. We defer our discussion of this to Sec. V. However, we make the important observation that if the system is close-packed to maximal density, then prescribing the position of the labeled part of any one agent determines the positions of the labeled parts of all other agents. Hence in the close-packed limit,

$$\mathbb{P}(\gamma_n(j) = 1,\, \gamma_n(j+L) = 1) = \mathbb{P}(\gamma_n(j) = 1) = \frac{1}{L}. \tag{13}$$

We now see that Eq. (12) is exactly correct in the close-packed limit. Since mean-field approximations are usually good in the low-density limit, having the correct high-density limit also opens the possibility of a good performance over the full range of densities.

It follows immediately from Eq. (11) that

$$\mathbb{P}(\gamma_n(j) = 0 \,|\, \gamma_n(j+L) = 1) \approx \frac{1 - L\mathbb{P}(\gamma_n(j) = 1)}{1 - (L-1)\mathbb{P}(\gamma_n(j) = 1)}. \tag{14}$$

A number of other equations that we need can be established by the same basic arguments. Suppose we know that site $(j+1)$ is completely vacant rather than occupied by the left-hand end of an agent. Since $\gamma_n(j+1) = 0$ means only that site $(j+1)$ is not occupied by the rightmost end of an agent, we express the state where site $(j+1)$ is completely vacant, with the indicator function $\gamma_n(j+s) = 0$ for $1 \le s \le L$, so that

$$\mathbb{P}(\gamma_n(j) = 1 \,|\, \gamma_n(j+s) = 0 \quad \text{for} \quad 1 \le s \le L) \approx \frac{\mathbb{P}(\gamma_n(j) = 1)}{1 - (L-1)\mathbb{P}(\gamma_n(j) = 1)} \tag{15}$$

and

$$\mathbb{P}(\gamma_n(j) = 0 \,|\, \gamma_n(j+s) = 0 \quad \text{for} \quad 1 \le s \le L) \approx \frac{1 - L\mathbb{P}(\gamma_n(j) = 1)}{1 - (L-1)\mathbb{P}(\gamma_n(j) = 1)}. \tag{16}$$

Since the choice of end to label is not an intrinsic part of the model we must make the approximations symmetrically should we know that site $j - L$ is either occupied or completely vacant of any part of an agent. We also make the approximation that $\gamma_n(j)$ and $\gamma_n(k)$ are independent if $|j - k| > L$.

We can now return to Eq. (10) and replace the compound probabilities iteratively with products of conditional probabilities. Recalling that $\gamma_n(i) = 1$ guarantees that $\gamma_n(i+s) = 0$ for $1 \leqslant s \leqslant L-1$ we have

$$\mathbb{P}(\gamma_n(i) = 1,\, \gamma_n(i+s) = 0 \quad \text{for} \quad L \le s \le d+L-1)$$

$$= \mathbb{P}(\gamma_n(i) = 1)\mathbb{P}(\gamma_n(i+s) = 0 \quad \text{for} \quad L \le s \le d+L-1 \,|\, \gamma_n(i) = 1,\, \gamma_n(i+s) = 0 \quad \text{for} \quad 1 \le s \le L-1) \tag{17}$$

$$= \mathbb{P}(\gamma_n(i) = 1) \prod_{s=1}^{d} \mathbb{P}(\gamma_n(i+L-1+s) = 0 \,|\, \gamma_n(i) = 1,\, \gamma_n(i+s') = 0 \quad \text{for} \quad 1 \le s' \le L+s-2). \tag{18}$$

Again, because $\gamma_n(i) = 1$ guarantees that $\gamma_n(i+s) = 0$ for $1 \leqslant s \leqslant L-1$, the $s = 1$ factor in the product is just $\mathbb{P}(\gamma_n(i+L) = 0 \,|\, \gamma_n(i) = 1)$ and so is given by the reflection-symmetric companion of Eq. (14). We use our approximation that $\gamma_n(j)$ and $\gamma_n(k)$ are independent if $|j - k| > L$ to evaluate the remaining factors (namely, $2 \leqslant s \leqslant d$) in the product. In the event on which the probability is conditioned, the requirements that $\gamma_n(i) = 1$ and $\gamma_n(i+s') = 0$ for $1 \leqslant s' \leqslant L+s-2$ can be

dropped, and then the reflected version of Eq. (16) can be used, giving

$$\mathbb{P}(\gamma_n(i)=1,\ \gamma_n(i+s)=0 \quad \text{for} \quad L\le s\le d+L-1) \approx \mathbb{P}(\gamma_n(i)=1)\prod_{s=1}^{d}\frac{1-L\,\mathbb{P}(\gamma_n(i+L-1+s)=1)}{1-(L-1)\,\mathbb{P}(\gamma_n(i+L-1+s)=1)}. \tag{19}$$

We deal with the other terms on the right in Eq. (10) similarly and deduce the master equation,

$$\begin{aligned}\mathbb{P}(\gamma_{n+1}(i)=1)-\mathbb{P}(\gamma_n(i)=1) = &-\frac{P}{2N}\mathbb{P}(\gamma_n(i)=1)\prod_{s=1}^{d}\frac{1-L\,\mathbb{P}(\gamma_n(i-L+1-s)=1)}{1-(L-1)\,\mathbb{P}(\gamma_n(i-L+1-s)=1)}\\ &-\frac{P}{2N}\mathbb{P}(\gamma_n(i)=1)\prod_{s=1}^{d}\frac{1-L\,\mathbb{P}(\gamma_n(i+L-1+s)=1)}{1-(L-1)\,\mathbb{P}(\gamma_n(i+L-1+s)=1)}\\ &+\frac{P}{2N}\mathbb{P}(\gamma_n(i+d)=1)\prod_{s=1}^{d}\frac{1-L\,\mathbb{P}(\gamma_n(i-L+s)=1)}{1-(L-1)\,\mathbb{P}(\gamma_n(i-L+s)=1)}\\ &+\frac{P}{2N}\mathbb{P}(\gamma_n(i-d)=1)\prod_{s=1}^{d}\frac{1-L\,\mathbb{P}(\gamma_n(i+L-s)=1)}{1-(L-1)\,\mathbb{P}(\gamma_n(i+L-s)=1)}.\end{aligned} \tag{20}$$

B. Continuum limit

The continuum limit is taken in exactly the same way is used in Sec. II B, where now $C(x,t)$ is a continuous variable representing the local average occupancy by the *rightmost end* of agents [so that $\mathbb{P}(\gamma_n(i)=1)=C(x,t)$ in the continuous limit]. The Taylor expansion in Eq. (5) is used again.

Since we are now considering agents occupying more than one site, at most one of every L consecutive sites can be occupied by the rightmost end of an agent at any one time. Therefore $C=C_{\max}=1/L$ corresponds to close-packed agents of length L.

As Eq. (20) is an explicit master equation that approximates the change in probability of occupancy at site i, we can take the continuum limit very easily. In the limit $\Delta,\tau\to 0$, with the ratio Δ^2/τ kept constant, Eq. (20) becomes the nonlinear diffusion equation

$$\frac{\partial C}{\partial t}=D_0\,\frac{\partial}{\partial x}\left(\mathcal{D}(C)\frac{\partial C}{\partial x}\right), \tag{21}$$

where D_0 is defined in Eq. (9) and

$$\frac{\mathcal{D}(C)}{d^2}=\frac{(1-L\,C)^{d-1}}{(1-(L-1)\,C)^{d+1}}(1+L(L-1)\,C^2). \tag{22}$$

Even though we are considering the case $L\ge 2$, we note that when $L=1$, Eqs. (21) and (22) reduce to Eqs. (7) and (8) since all terms with an $(L-1)$ factor vanish.

Unlike previous papers in this area [5–8], the diffusivity we have obtained is not a polynomial: it is a rational function in C arising from the fractional nature of our approximations. The diffusivity at maximum density, $\mathcal{D}(1/L)$, is zero provided $d>1$, as it was for the $L=1$ case in Sec. II.

As in Sec. II, the diffusivity scales with d^2, as any movement always occurs over a distance $d\Delta$. We therefore consider $\mathcal{D}(C)/d^2$. We can rewrite Eq. (22) as a Taylor series in C and obtain the equivalent equation

$$\frac{\mathcal{D}(C)}{d^2}=1+(2L-d-1)C+O(C^2). \tag{23}$$

We can therefore see that the scaled diffusivity increases with C at low densities if $2L>d+1$, and decreases as C increases if $2L<d+1$. Figure 4(a) illustrates several examples of the first case (all with $d=L$ and so $2L>d+1$ for $d,L>1$), where the scaled diffusivity initially increases, while Fig. 4(b) illustrates several examples of the second case (all with $d=2L$ and so $2L<d+1$), where the scaled diffusivity initially decreases.

We vary both L and d and so can consider the effects of increasing both while keeping the ratio between them constant: effectively reducing the lattice size for agents of fixed size. We therefore consider $\mathcal{D}(C)/d^2$ and present an example for the case $L=d$. Rearranging Eq. (22) gives

$$\frac{\mathcal{D}(C)}{d^2}=\frac{(1-\widetilde{C})^{d-1}}{(1-s\,\widetilde{C})^{d+1}}(1+s\,\widetilde{C}^2),\quad 0\le\widetilde{C}\le 1, \tag{24}$$

where $\widetilde{C}=C/C_{\max}$, $s=(d-1)/d$, and $C_{\max}=1/L$. Figure 4(a) illustrates this behavior; as d increases, the scaled diffusivity increases at medium densities but decreases at high densities, with zero diffusivity at the maximum density for all $d>1$. Figure 4(b) shows the equivalent behavior when $d=2L$.

We can see from Fig. 4 that the scaled diffusivity is nonmonotonic in $\widetilde{C}$ when $d=L$, while the corresponding diffusivity decreases monotonically when $d=2L$. This is an interesting result for which we do not have a physically intuitive argument.

C. Simulations

Simulations are performed using MATLAB on a lattice with $1\le x\le 200\,d$ and either dimer agents ($L=2$) or agents occupying four sites ($L=4$) initially placed in the center of the lattice at half the maximum possible density (see Appendix). We consider two examples: one where agents attempt to move in steps of two lattice sites and another where agents attempt to move in steps of four lattice sites. Figure 5 compares averaged simulation data and solutions of the PDE description [Eqs. (21) and (22)]. We see that the agent occupancy C is well described by the PDE solutions. Results for longer agents were of a

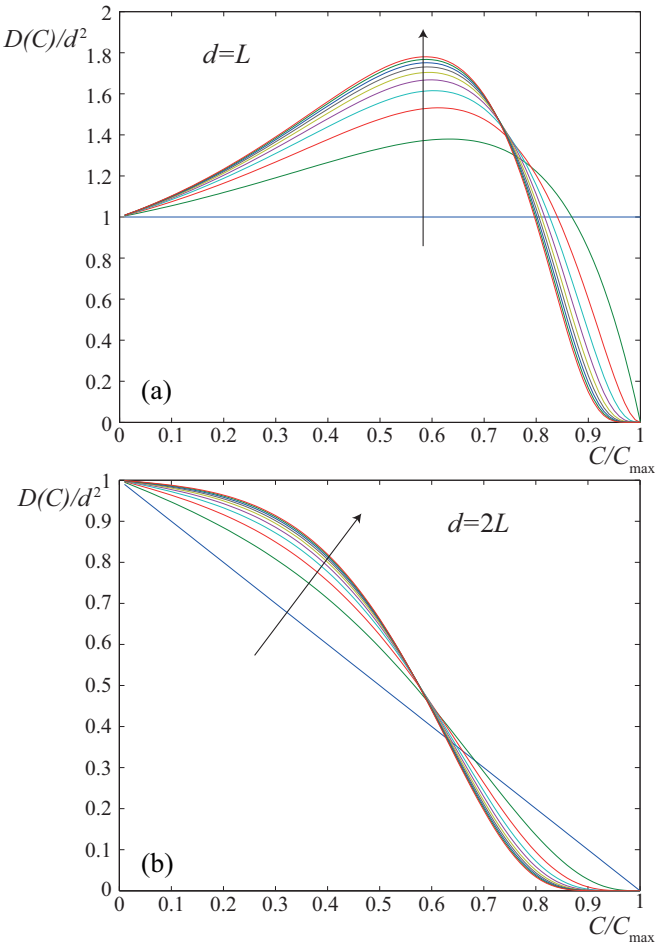

FIG. 4. (Color online) Fixed movement distance. The diffusion coefficient scaled with fixed distance d, and $\mathcal{D}(C)/d^2$ given by Eq. (24), for two ratios of L and d: (a) $d = 1, \ldots, 10$ and $L = d$ and (b) $d = 2, \ldots, 20$ and $L = \frac{1}{2}d$. Black arrows indicate increasing d and $C_{\max} = 1/L$. Note the different scales on the vertical axes.

similar quality, including agents with $L = 10$ moving longer distances including $d = 10$ (not shown here).

The regular oscillations (observed when $L = 1$ in Fig. 3) do not appear when $L = d = 2$ in Fig. 5 because the longer agents are not moving distances more than their length. As d increases for any given L, the oscillations reappear as observed in the simulations when $L = 2$ and $d = 4$ (Fig. 5).

The unusual shape of the initial condition for the simulations in Fig. 5 is due to the difficulties of randomly generating positions for longer agents. Once some agents have been randomly placed and so some positions are no longer available, agents are more or less likely to fit near the boundaries (depending on whether or not the agents are allowed to overlap the edges) and so produce the unusual shape.

IV. INTEGER LENGTH AGENTS MOVING UP TO A FIXED DISTANCE

Consider the case where agents may not be able to move the full distance d. Now they are permitted to move as far as possible until prevented from moving farther by the presence of another agent. Each agent has a length $L\Delta$ for some positive integer L and moves a distance up to $d\Delta$ along the lattice. This change in the rules allows the agents to move more often, on average, on a more densely packed lattice.

A. Probabilistic model

We use the same one-dimensional lattice as in Sec. III, with the same probabilities of movement and indicator variable, except that now an agent can move at least one lattice site in a given direction as long as its immediate neighboring site is empty. There are now six ways a single agent move of a monomeric agent ($L = 1$) can change the occupancy of any given site i: two by vacating i and four by moving into i. An agent already at i can vacate it either by moving left, if at least site $i - 1$ is empty, or by moving right, if at least site $i + 1$ is empty. If site i is empty, an agent at site $i + d$ moving to the left occupies site i if all of the intermediate sites are empty and an agent at site $i - d$ moving to the right occupies site i if all of the intermediate sites are empty. An empty site i can also become occupied if site $i + 1$ is occupied and the closest agent less than d sites to the left moves right (it attempts to move farther but cannot, as the agent at site $i + 1$ is in the way) or, if site $i - 1$ is occupied, the closest agent less than d sites to the right can move left into site i. An example of the latter kind of occupancy change is shown in Fig. 6.

More generally, when $L > 1$, there are also six ways in which a single move by an agent can change the right-end occupancy status of a single site. This change in the movement rules modifies Eq. (10). Instead, the probability that site i is occupied by the rightmost end of an agent at time step $n + 1$ is given by

$$
\begin{aligned}
&\mathbb{P}(\gamma_{n+1}(i) = 1) - \mathbb{P}(\gamma_n(i) = 1) \\
&\quad = -\frac{P}{2N}\mathbb{P}(\gamma_n(i) = 1,\ \gamma_n(i - L) = 0) - \frac{P}{2N}\,\mathbb{P}(\gamma_n(i) = 1,\ \gamma_n(i + L) = 0) \\
&\qquad + \frac{P}{2N}\,\mathbb{P}(\gamma_n(i + d) = 1,\ \gamma_n(i + s) = 0 \quad \text{for} \quad 1 - L \le s \le d - L) \\
&\qquad + \frac{P}{2N}\,\mathbb{P}(\gamma_n(i - d) = 1,\ \gamma_n(i - s) = 0 \quad \text{for} \quad 1 - L \le s \le d - L) \\
&\qquad + \frac{P}{2N}\,(\mathbb{P}(\gamma_n(i + L) = 1,\ \gamma_n(i) = 0) - \mathbb{P}(\gamma_n(i + L) = 1,\ \gamma_n(i - s) = 0 \quad \text{for} \quad 0 \le s \le d - 1)) \\
&\qquad + \frac{P}{2N}\,(\mathbb{P}(\gamma_n(i - L) = 1,\ \gamma_n(i) = 0) - \mathbb{P}(\gamma_n(i - L) = 1,\ \gamma_n(i + s) = 0 \quad \text{for} \quad 0 \le s \le d - 1)).
\end{aligned}
\tag{25}
$$

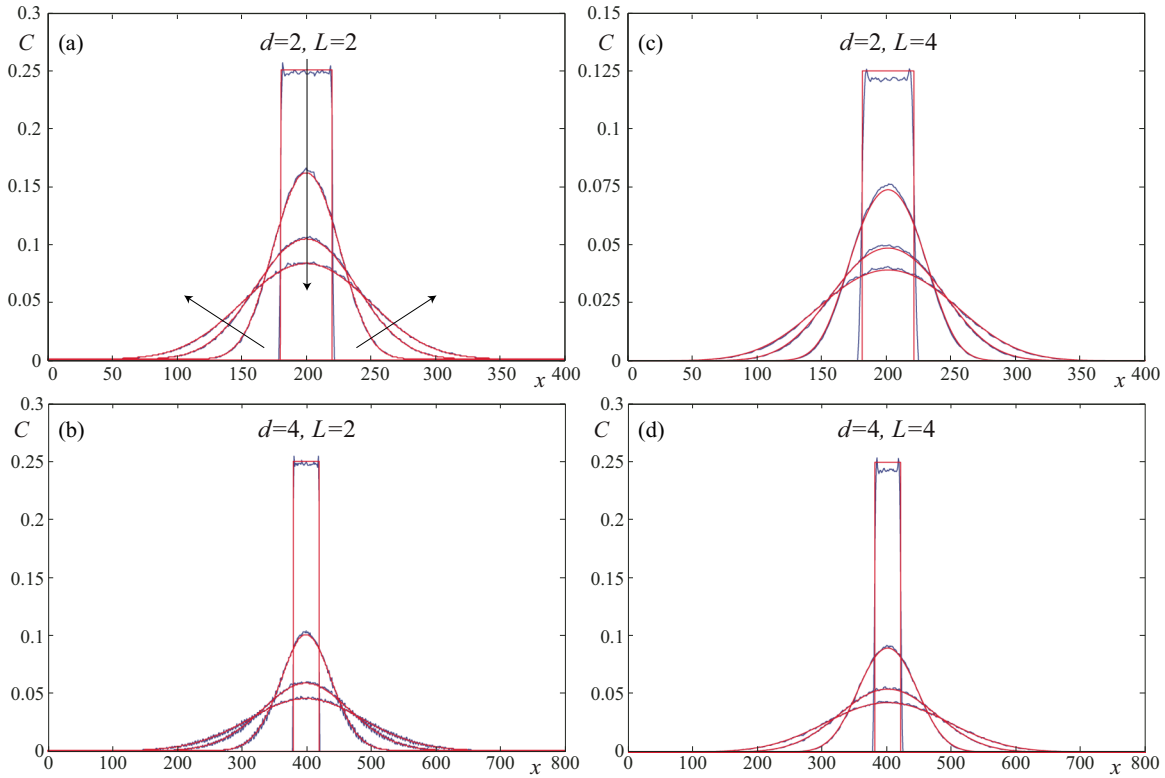

FIG. 5. (Color online) Dimer agents (i.e., $L = 2$) and agents occupying four sites ($L = 4$) moving exactly d lattice sites: Solutions to Eq. (21) [medium-gray (red) curves] for $d = 2$ and 4 compared to the average of 50 000 simulations [dark-gray (blue) curves] at times $t = 100$, 300, and 500. The initial condition is also shown, with agents between $181 \leqslant x \leqslant 220$ for $d = 2$ and between $381 \leqslant x \leqslant 420$ for $d = 4$. Note the different scales on the x axes: for larger values of d the outermost agents move farther, and so a larger region is needed to prevent interference with the boundaries or $t \leqslant 500$. Equations (21) and (22) are solved using MATLAB **pdepe** with $\delta x = 0.1$. Arrows in (a) indicate increasing time.

We make the same approximations as in Sec. III, given in Eqs (11) and (15), to produce the master equation:

$$
\begin{aligned}
&\mathbb{P}(\gamma_{n+1}(i)=1)-\mathbb{P}(\gamma_n(i)=1)\\
&=\frac{P}{2N}\left\{-\mathbb{P}(\gamma_n(i)=1)\left(\frac{1-L\,\mathbb{P}(\gamma_n(i-L)=1)}{1-(L-1)\,\mathbb{P}(\gamma_n(i-L)=1)}+\frac{1-L\,\mathbb{P}(\gamma_n(i+L)=1)}{1-(L-1)\,\mathbb{P}(\gamma_n(i+L)=1)}\right)\right.\\
&\quad+\mathbb{P}(\gamma_n(i+d)=1)\prod_{s=1}^{d}\frac{1-L\,\mathbb{P}(\gamma_n(i-L+s)=1)}{1-(L-1)\,\mathbb{P}(\gamma_n(i-L+s)=1)}\\
&\quad+\mathbb{P}(\gamma_n(i-d)=1)\prod_{s=1}^{d}\frac{1-L\,\mathbb{P}(\gamma_n(i+L-s)=1)}{1-(L-1)\,\mathbb{P}(\gamma_n(i+L-s)=1)}\\
&\quad+\mathbb{P}(\gamma_n(i+L)=1)\left(\frac{1-L\,\mathbb{P}(\gamma_n(i)=1)}{1-(L-1)\,\mathbb{P}(\gamma_n(i)=1)}-\prod_{s=0}^{d-1}\frac{1-L\,\mathbb{P}(\gamma_n(i-s)=1)}{1-(L-1)\,\mathbb{P}(\gamma_n(i-s)=1)}\right)\\
&\quad\left.+\mathbb{P}(\gamma_n(i-L)=1)\left(\frac{1-L\,\mathbb{P}(\gamma_n(i)=1)}{1-(L-1)\,\mathbb{P}(\gamma_n(i)=1)}-\prod_{s=0}^{d-1}\frac{1-L\,\mathbb{P}(\gamma_n(i+s)=1)}{1-(L-1)\,\mathbb{P}(\gamma_n(i+s)=1)}\right)\right\}. \qquad (26)
\end{aligned}
$$

B. Continuum limit

The continuum limit uses the same techniques and notation as described previously. Exactly as in Sec. III, we use Taylor expansions to analyze Eq. (26) in the limit $\Delta, \tau \to 0$, keeping the ratio Δ^2/τ constant. We obtain the nonlinear diffusion equation

$$
\frac{\partial C}{\partial t} = D_0 \frac{\partial}{\partial x}\left(\mathcal{D}(C)\frac{\partial C}{\partial x}\right), \qquad (27)
$$

FIG. 6. (Color online) Movement up to a fixed distance d, illustrated for a monomeric agent. For any $d \geqslant 3$, the right [open (blue) circle] agent will occupy the green (light gray) site if it attempts to move left, since the left [open (red) circle] agent prevents any further movement.

where D_0 is defined in Eq. (9) and

$$\mathcal{D}(C) = \frac{L^2[1-2(L-1)C+L(L-1)C^2]}{(1-(L-1)C)^2} + \frac{(d-L)(1-LC)^{d-1}}{(1-(L-1)C)^{d+1}}\big[d+L-L(d+2L-1)C + L(L-1)(d+L)C^2\big]. \tag{28}$$

The diffusivity $\mathcal{D}(C)$, like the equivalent expression in Sec. III for fixed distance movement, is a rational function in C. Since movement can occur at much closer distances than d lattice sites, the d^2 factor in the diffusivity disappears. We note that when $d = 1$, the diffusivity expression in Eq. (28) reduces to the one in Eq. (22), as expected. In addition, when $L = 1$ the expression for $\mathcal{D}(C)$ simplifies to

$$\mathcal{D}(C) = 1 + (d^2-1)(1-C)^d. \tag{29}$$

Unlike the diffusivity for movement over a fixed distance found in Sec. III B, here, when $d > 1$, the diffusivity does not decrease to zero at the maximum density, but $\mathcal{D}(1) = 1$. This has an intuitive explanation since at a high density, it is unlikely that there are d consecutive empty sites, when $d \geq 2$. Therefore agents in this model can move into a vacant neighboring site, while agents in Sec. III, would have their attempted moves aborted unless there are d consecutive empty sites.

We again consider the scaled diffusivity $\mathcal{D}(C)/d^2$ and rewrite Eq. (28) as a Taylor series in C. We obtain the equivalent equation

$$\frac{\mathcal{D}(C)}{d^2} = 1 + \frac{(L-d)(d+1)}{d}C + O(C^2). \tag{30}$$

We can therefore see that the scaled diffusivity increases with C at low densities if $d < L$ and decreases as C increases if $d > L$. If $d = L$, we expect the scaled diffusivity to remain near 1. Figure 7 shows several examples of all three possibilites: $d < L$ and the scaled diffusivity increases in Fig. 7(a), $d = L$ and the scaled diffusivity changes very slowly in Fig. 7(b), and $d > L$ and the scaled diffusivity initially decreases in Fig. 7(c).

As in Sec. III, we look at the scaled diffusivity for a fixed ratio of L and d. When $L = d$ the factor $(d - L) = 0$ and so Eq. (28) can be rearranged as

$$\frac{\mathcal{D}(C)}{d^2} = \frac{1 - s\,\widetilde{C}\,(2-\widetilde{C})}{(1-s\,\widetilde{C})^2}, \quad 0 \leq \widetilde{C} \leq 1, \tag{31}$$

where $\widetilde{C} = C/C_{\max}$, $s = (d-1)/d$, and $C_{\max} = 1/L$. Figure 7(b) illustrates this for various values of d. As d increases the diffusivity close to maximum density now increases since agents can move a small distance whenever there is any empty space.

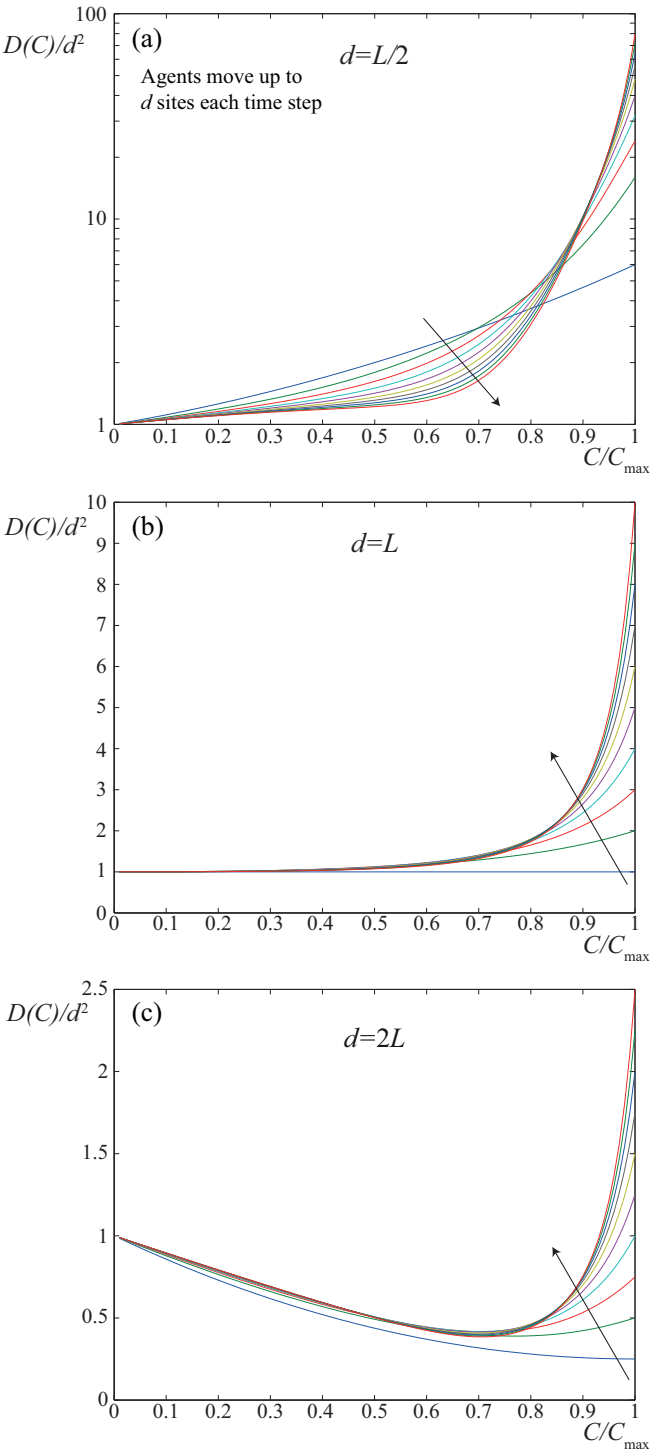

FIG. 7. (Color online) Movement up to a distance d. The diffusion coefficient scaled with distance $\mathcal{D}(C)/d^2$, given by Eq. (31), for three ratios of L and d: (a) $d = 1, \ldots, 10$ and $L = 2d$, (b) $d = 1, \ldots, 10$ and $L = d$, and (c) $d/2 = 1, \ldots, 10$ and $L = \frac{1}{2}d$. Black arrows indicate increasing d, and in all cases $C_{\max} = 1/L$. Note the different scales on the y axis: the scaled diffusivity is much larger at maximum density when L is large compared to d. Also, note the logarithmic scale in (a).

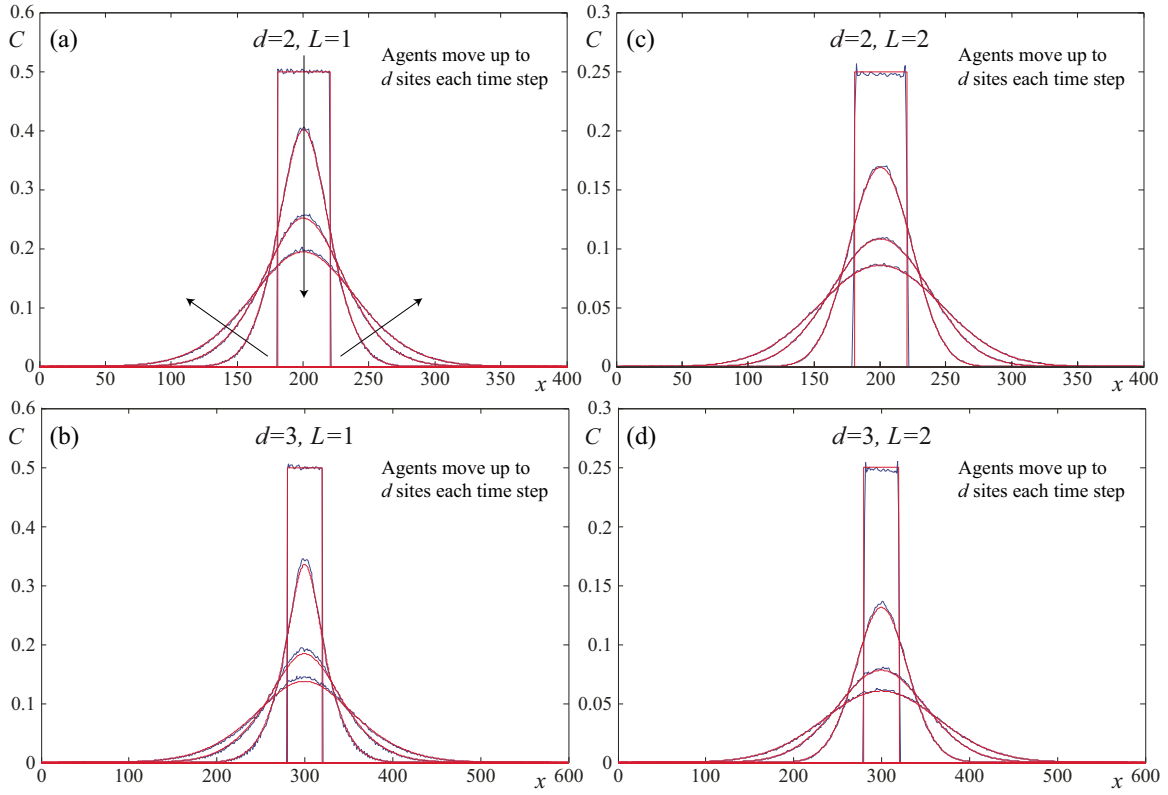

FIG. 8. (Color online) Monomer agents ($L = 1$) and dimer agents ($L = 2$) moving up to d lattice sites: Solutions to Eq. (27) [medium-gray (red) curves] compared to the average of 50 000 simulations [dark-gray (blue) curves] at times $t = 100$, 300, and 500. (a) $L = 1$ and $d = 2$; (b) $L = 1$ and $d = 3$; (c) $L = 2$ and $d = 2$; (d) $L = 2$ and $d = 3$. The initial condition (shown) has agents between $181 \leqslant x \leqslant 220$ for $d = 2$ and agents between $281 \leqslant x \leqslant 320$ for $d = 3$. Note the different scales on the x axis: for larger values of d the outermost agents move farther, and so a larger region is needed to prevent interference with the boundaries for $t \leqslant 500$. Equations (27) and (28) were solved using MATLAB **pdepe** with $\delta x = 0.1$. Arrows in (a) indicate increasing time.

C. Simulations

Simulations are performed on a lattice with $1 \leq x \leq 200\,d$ and agents initially placed in the center of the lattice at half-density (see Appendix). Figure 8 compares the average over many simulations with the solution to the nonlinear diffusion equation (27) with diffusivity given by Eq. (28) for monomer agents ($L = 1$) and dimer agents ($L = 2$) for $d = 2$ and $d = 3$. There is a very good match between the average simulation results and the PDE solutions, although small differences appear in the center as d increases. These slight differences, which persist for longer agents and increase for the highest agent density, are due to errors in the approximations: since agents can move until they are prevented by the presence of another agent, agents are more likely to be neighboring each other than separated by an empty lattice site, but our approximations do not take this into account. For most agent densities the differences are small, even when the agents are large.

Unlike the examples in Sec. II, there are very few of the persistent oscillations towards the edges of the simulation. As agents are no longer forced to move exactly d spaces each time, they will not always remain on the same set of sites d spaces apart.

V. DISCUSSION

When monomers move only to their nearest-neighbor sites, without directional bias and using simple exclusion rules, it is well known that the agents collectively exhibit linear diffusion: this is both the prediction of mean-field theory, confirmed by simulation [5,11,14], and a rigorously established result [1,17]. Our work here allows a general extension to monomer agents ($L = 1$) that can attempt to move an integer distance d each time step in one dimension. Collectively, such agents satisfy a nonlinear diffusion equation. In the case where agents move exactly d sites or not at all, the diffusion coefficient is given by

$$\mathcal{D}(C) = d^2(1 - C)^{d-1}.$$

When agents move up to d sites or until blocked by the presence of another agent, the diffusion coefficient is given by

$$\mathcal{D}(C) = 1 + (d^2 - 1)(1 - C)^d.$$

In both models the increase in movement distance allows greater diffusivity at lower densities, although when the distance d is fixed, higher densities provide a greater chance that agents will be prevented from moving and so decreases the diffusivity.

We have shown that when the agents have length $L > 1$, satisfying the simplest type of interaction, namely, simple exclusion, when only nearest-neighbor moves are permitted ($d = 1$), the diffusivity is no longer a polynomial but is now a rational function of C, namely,

$$\mathcal{D}(C) = \frac{1 + L(L-1)\,C^2}{(1 - (L-1)\,C)^2}.$$

This is an unusual result, as previous theory, covering a general class of interacting lattice-based monomer agents which move to nearest-neighbor sites, always generates a nonlinear diffusion equation where the associated diffusivity is a polynomial in C which can be determined explicitly [5].

For the most general case where $L > 1$ and $d > 1$, agents collectively exhibit nonlinear diffusion, where the diffusivity is a rational function of C, when the distance moved by an agent is d or up to d lattice spacings. The diffusivity we have obtained is zero at the maximum possible density for fixed distance steps of more than one lattice site (i.e., $d > 1$), while this is not the case when agents can make partial steps if they are blocked from moving the full distance.

Our observations regarding the shape of the diffusion coefficient and their values at maximum density should not be overinterpreted since the agent movement depends on the flux, which is a product of two terms:

$$J = -\mathcal{D}(C)\nabla C.$$

Close to the maximum density the gradient in the local agent occupancy will be very small, so it is not necessary to have $\mathcal{D}(C)$ small to turn off the flux.

Furthermore, we should distinguish between self-diffusion of a single tagged agent in a collection of similarly moving agents and the population-level diffusivity. As an example, consider the case $L = 1, d = 1$ [14]. The mean-squared displacement of a single agent in a simple exclusion process is proportional to $D_0(1 - C)$ so decreases linearly with C due to crowding. However, when the continuum limit of the master equation is taken, the corresponding PDE has a diffusive flux term, namely, $-D_0(1 - C)\nabla C$, and a convective flux term proportional to $-D_0 C\nabla C$. The two together cancel the nonlinear term, producing a net flux of $-D_0\nabla C$, thus producing the linear diffusion equation given in Eq. (7). This demonstrates that the intuitive expectation that the diffusivity decreases with crowding is false, as it remains a constant in the most simple case examined here.

The determined PDEs provide a very good model for the collective behavior at both low and high densities. The PDE continues to model the collective motion well for significantly longer agents; we have tested the results up to $L = 10$.

The increase in accuracy of our results compared to previous work is due to the improved approximations we make to extend the mean field beyond monomer agents. In our previous paper [15] when studying the movement of dimer agents ($L = 2$) we used the approximation that the occupancies of two sites at least L lattice sites apart were independent. Figure 9 compares the two approximations: the approximation that lattice sites a distance L apart are independent and the approximations used in this paper and described in Eq. (11), that the relative probabilities that a site will be occupied or completely vacant are unchanged by the knowledge that there is an agent in the neighboring position L lattice sites away. It is possible to use the alternative approximations to obtain a nonlinear diffusion equation which describes the movement of agent with any length moving any distance [18], but since the approximations become increasingly inaccurate for longer agents [shown clearly in Fig. 8(b) for agents with $L = 5$], this produces a result worse than the one we have detailed here.

This paper represents a significant advance over previous work on lattice-based polymeric agents [6,7,15] (which addressed linear polymeric agents). A difficulty with implanting mean-field ideas for nonmonomeric agents is that there are several ways to perform the calculation and some ways can yield unphysical results at low densities. Of particular importance is the careful assessment of mean-field arguments from a properly enunciated probability viewpoint, which enables appropriate mean-field approximations to be identified more easily for polymeric agents. Also, we compare and contrast motility rules that abort attempted steps when any obstacle intervenes with motility rules that accept a smaller translation less than d if another agent intrudes. Our mean-field approximations are tested, shown to be highly accurate, and validated against simulations.

In this paper we have considered agents moving on a one-dimensional lattice. It would be possible to extend this to movement on higher dimensional lattices, either with movement over larger distances in a straight line or by allowing agents to move more than one lattice space in different directions. For agents occupying more than one site,

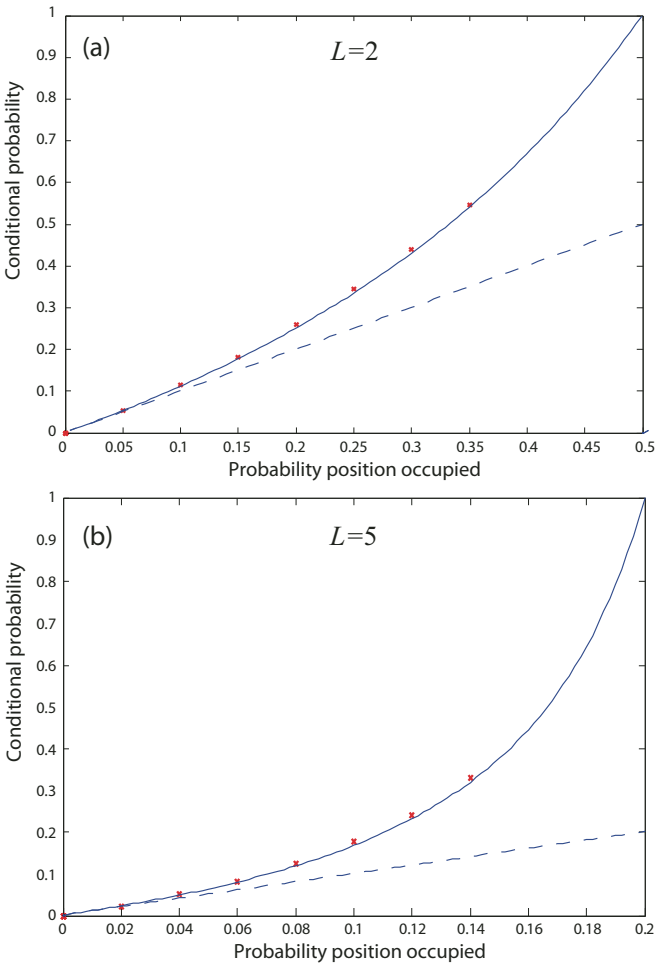

FIG. 9. (Color online) Comparison of approximations: Eq. (11) [solid (blue) line] compared to simulations [(red) crosses] and the approximation that the occupancies of any two lattice sites at least L lattice sites apart are independent [dashed (blue) line], for (a) $L = 2$ and (b) $L = 5$. Simulated results are not shown for high densities due to the difficulties of placing long agents randomly. Note the different scales on the x axis: agents of different lengths result in different maximum densities.

there are several alternative models: either the agents are (approximately) spherical in space and so have no orientation or they are longer in one direction than the other and the model has to involve some method of changing orientations [6,15].

By decoupling the agent size (linear polymers of arbitrary length L) and the step distance (d), we are able to approximate an off-lattice process, as steps are no longer integer multiples of agent size. We explored the effects of increasing the agent length L and movement distance d, while maintaining the same ratio between L and d. This is a useful starting point for further investigations.

ACKNOWLEDGMENT

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APPENDIX: SIMULATION DETAILS

All simulations are performed using MATLAB on a lattice with $1 \leq x \leq 200\,d$. The N agents are initially randomly placed in a region 40 sites wide in the center of the lattice, $100\,d - 19 \leqslant x \leqslant 100\,d + 20$. The number of agents N is chosen so that this central region is initially occupied at half the maximum density: where the agent density is sufficiently high for some agent movements to be blocked by the presence of other agents but not so high that most movements are aborted. The simulations are implemented with zero-flux boundary conditions, although the lattice sizes are chosen to be large enough that agents are extremely unlikely to reach the lattice boundaries. In all simulations, we use $P = 1$, $\Delta = 1$, and $\tau = 1$.

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[16] For each possible change in occupancy to occur, we require three conditions, reflected in each term on the right-hand side of Eq. (1): (i) there must be an agent at the appropriate position; (ii) that agent must be chosen to move in the appropriate direction; and (iii) there must be no other agents between the agent and its destination or the move will be aborted. Therefore, for example, the probability that the occupancy of site i changes because an agent already at i moves left to vacate it is

$$\begin{aligned}&\mathbb{P}(\text{an agent at } i \text{ moves left})\\ &= \mathbb{P}\begin{pmatrix}\gamma_n(i) = 1 \text{ and it is chosen to move left}\\ \text{and } \gamma_n(i-s) = 0 \quad \text{for} \quad 1 \leqslant s \leqslant d\end{pmatrix}\\ &= \frac{P}{2N}\mathbb{P}(\gamma_n(i) = 1, \gamma_n(i-s) = 0 \quad \text{for} \quad 1 \leqslant q \leqslant d),\end{aligned}$$

since the chance of any agent being chosen to move is P/N, independent of its surroundings, and agents attempt to move in each direction with equal probability.

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