Diffusion of tagged particles in a crowded medium: supplementary material. Paper submitted to Europhys. Lett.

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I. DERIVATION OF THE MEAN FIELD EQUATIONS IN TWO DIMENSION

As stated in the main text, the equations governing the evolution of the particles, which we obtained for a $1D$ setting, can be extended to higher dimensions. In the following we will provide a detailed derivation for the mean field equations in $2D$. We will first generalized the procedure described in the main body of the paper and then turn to consider and alternative approach inspired to the work of Landman and collaborators (see e.g. Simpson, Landman and Hughes Phys Rev E 79 031920 (2009)).

To progress in the analysis we assume each site of the the two-dimensional lattice to be labelled with two indices (i, j). In the $2D$ case, the nearest neighbour sites the selected particle can jump to are four. This is at variance with the 1D geometry where each site has just two adjacent neighbors. The binary variables at time k are hence indicated as $m_{i,j}(k)$ and $n_{i,j}(k)$.

The stochastic process reads:

$$
\begin{aligned}
m_{i,j}(k+1) - m_{i,j}(k) \;=\;& z^+_{i-1} m_{i-1,j}(k)[1 - m_{i,j}(k)][1 - n_{i,j}(k)] + z^-_{i+1} m_{i+1,j}(k)[1 - m_{i,j}(k)][1 - n_{i,j}(k)] \\
&+ z^+_{j-1} m_{i,j-1}(k)[1 - m_{i,j}(k)][1 - n_{i,j}(k)] + z^-_{j+1} m_{i,j+1}(k)[1 - m_{i,j}(k)][1 - n_{i,j}(k)] \\
&- z^+_i m_{i,j}(k)[1 - m_{i+1,j}(k)][1 - n_{i+1,j}(k)] - z^-_i m_{i,j}(k)[1 - m_{i-1,j}(k)][1 - n_{i-1,j}(k)] \\
&- z^+_i m_{i,j}(k)[1 - m_{i,j+1}(k)][1 - n_{i,j+1}(k)] - z^-_i m_{i,j}(k)[1 - m_{i,j-1}(k)][1 - n_{i,j-1}(k)]
\end{aligned} \tag{1}
$$

where the stochastic variables $z^\pm$ are defined in analogy to the one dimensional case. The equation governing the evolution of $n_{i,j}(\cdot)$ can be equivalently modified. After introducing the one-body occupancy probabilities

$$\rho_{i,j}(k) = \langle\langle m_{i,j}(k)\rangle\rangle \tag{2}$$

$$\phi_{i,j}(k) = \langle\langle n_{i,j}(k)\rangle\rangle \tag{3}$$

and assuming a mean-field factorization for the two-body and three-body correlations, one eventually ends up with

$$
\begin{aligned}
\rho_{i,j}(k+1) - \rho_{i,j}(k) \;=\;& q\left(\rho_{i-1,j}(k) + \rho_{i+1,j}(k) + \rho_{i,j-1}(k) + \rho_{i,j+1}(k)\right)[1 - \rho_{i,j}(k)]\,[1 - \phi_{i,j}(k)] \\
&- q\,\rho_{i,j}(k)[4 - (\rho_{i-1,j}(k) + \rho_{i+1,j}(k)) - (\rho_{i,j-1}(k) + \rho_{i,j+1}(k)) - (\phi_{i-1,j}(k) + \phi_{i+1,j}(k)) \\
&- (\phi_{i,j-1}(k) + \phi_{i,j+1}(k+1)) + \phi_{i+1,j}(k)\rho_{i+1,j}(k) + \phi_{i-1,j}(k)\rho_{i-1,j}(k) + \phi_{i,j+1}(k)\rho_{i,j+1}(k) \\
&+ \phi_{i,j-1}(k)\rho_{i,j-1}(k)]
\end{aligned} \tag{4}
$$

$$
\begin{aligned}
\phi_{i,j}(k+1) - \phi_{i,j}(k) \;=\;& w\left(\phi_{i-1,j}(k) + \phi_{i+1,j}(k) + \phi_{i,j-1}(k) + \phi_{i,j+1}(k)\right)[1 - \phi_{i,j}(k)]\,[1 - \rho_{i,j}(k)] \\
&- w\,\phi_{i,j}(k)[4 - (\phi_{i-1,j}(k) + \phi_{i+1,j}(k)) - (\phi_{i,j-1}(k) + \phi_{i,j+1}(k)) - (\rho_{i-1,j}(k) + \rho_{i+1,j}(k)) \\
&- (\rho_{i,j-1}(k) + \rho_{i,j+1}(k)) + \phi_{i+1,j}(k)\rho_{i+1,j}(k) + \phi_{i-1,j}(k)\rho_{i-1,j}(k) + \phi_{i,j+1}(k)\rho_{i,j+1}(k) \\
&+ \phi_{i,j-1}(k)\rho_{i,j-1}(k)]
\end{aligned} \tag{5}
$$

Assume the concentration of the tagged particles to be small, namely $\rho_{i,j} \ll 1$. Then the following approximated relations are found:

$$\begin{aligned}
\rho_{i,j}(k+1) - \rho_{i,j}(k) &= q(\rho_{i-1,j}(k) + \rho_{i+1,j}(k) \\
&+ \rho_{i,j-1}(k) + \rho_{i,j+1}(k))\,[1 - \phi_{i,j}(k)] \\
&- q\rho_{i,j}(k)[4 - (\phi_{i-1,j}(k) + \phi_{i+1,j}(k) \\
&+ \phi_{i,j-1}(k) + \phi_{i,j+1}(k))] \\
\phi_{i,j}(k+1) - \phi_{i,j}(k) &= w(\phi_{i-1,j}(k) + \phi_{i+1,j}(k) - 2\phi_{i,j}(k) \\
&+ \phi_{i,j-1}(k) + \phi_{i,j+1}(k) - 2\phi_{i,j}(k))
\end{aligned}$$

After introducing the continuous variables

$$\rho(x,y,t) = \lim_{a,\Delta t \to 0} \rho_{i,j}(k), \qquad \phi(x,y,t) = \lim_{a,\Delta t \to 0} \phi_{i,j}(k) \tag{6}$$

where a andΔt respectively stand for the linear size of the lattice site and the characteristic time step of the microscopic dynamics. By defining the diffusion coefficients according to the standard practice (see main body of the paper), we get the sought generalized model:

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &= \nabla^2 \left[D_\rho (1-\phi)\rho\right] + 2D_\rho \nabla \cdot (\rho \nabla \phi) \\
\frac{\partial \phi}{\partial t} &= D_\phi \nabla^2 \phi
\end{aligned} \tag{7}$$

As anticipated, we shall now turn to discussing an alternative derivation of the above equation. To this end, we define the variable

$$\gamma_{i,j}(k) = \begin{cases} 1, & \text{if the site } (i,j) \text{ is occupied by an agent of the species } m \text{ at time step } k \\ 2, & \text{if the site } (i,j) \text{ is occupied by an agent of the species } n \text{ at time step } k \\ 0 & \text{if the site } (i,j) \text{ is empty at the time step } k \end{cases} \tag{8}$$

We write then the master equation for the motion of the tagged particles as:

$$\begin{aligned}
&\mathbb{P}^1(\gamma_{i,j}(k+1) = 1) - \mathbb{P}^1(\gamma_{i,j}(k) = 1) = -\alpha \Big[\mathbb{P}^2\Big(\gamma_{i,j}(k) = 1, \gamma_{i+1,j}(k) = 0\Big) + \mathbb{P}^2\Big(\gamma_{i,j}(k) = 1, \gamma_{i-1,j}(k) = 0\Big) \\
&+ \mathbb{P}^2\Big(\gamma_{i,j}(k) = 1, \gamma_{i,j+1}(k) = 0\Big) + \mathbb{P}^2\Big(\gamma_{i,j}(k) = 1, \gamma_{i,j-1}(k) = 0\Big)\Big] + \alpha \Big[\mathbb{P}^2\Big(\gamma_{i,j}(k) = 0, \gamma_{i+1,j}(k) = 1\Big) \\
&+ \mathbb{P}^2\Big(\gamma_{i,j}(k) = 0, \gamma_{i-1,j}(k) = 1\Big) + \mathbb{P}^2\Big(\gamma_{i,j}(k) = 0, \gamma_{i,j+1}(k) = 1\Big) + \mathbb{P}^2\Big(\gamma_{i,j}(k) = 0, \gamma_{i,j-1}(k) = 1\Big)\Big]
\end{aligned} \tag{9}$$

where $\mathbb{P}^2$ stands for a joint probability, while $\mathbb{P}^1$ is the probability of a single event and α is the rate of success of the selected jump. The master equation for the population n is similar, the variable γ assuming the value 2 instead of 1 and β labeling the associated jump rate (in principle the two population can have different jump probabilities). In the mean field limit, we factorize the joint probabilities $\mathbb{P}^2$ in the master equations as in

$$\mathbb{P}^2\big(\gamma_{i,j}(k) = 1, \gamma_{i,j+1}(k) = 0\big) = \\ \mathbb{P}^1\big(\gamma_{i,j}(k) = 1\big)\mathbb{P}^1\big(\gamma_{i,j+1}(k) = 0\big).$$

To perform the continuum limit we employ a Taylor expansion for the three different probability functions $\mathbb{P}^1$ as:

$$
\begin{aligned}
\mathbb{P}(\gamma_{i\pm1,j}(k)=1) &= \rho \pm a\frac{\partial\rho}{\partial x}+\frac{1}{2}a^2\frac{\partial^2\rho}{\partial x^2}+o(a^2)\\
\mathbb{P}(\gamma_{i,j\pm1}(k)=1) &= \rho \pm a\frac{\partial\rho}{\partial y}+\frac{1}{2}a^2\frac{\partial^2\rho}{\partial y^2}+o(a^2)\\
\mathbb{P}(\gamma_{i\pm1,j}(k)=2) &= \phi \pm a\frac{\partial\phi}{\partial x}+\frac{1}{2}a^2\frac{\partial^2\phi}{\partial x^2}+o(a^2)\\
\mathbb{P}(\gamma_{i,j\pm1}(k)=2) &= \phi \pm a\frac{\partial\phi}{\partial y}+\frac{1}{2}a^2\frac{\partial^2\phi}{\partial y^2}+o(a^2)\\
\mathbb{P}(\gamma_{i\pm1,j}(k)=0) &= \mu \pm a\frac{\partial\mu}{\partial x}+\frac{1}{2}a^2\frac{\partial^2\mu}{\partial x^2}+o(a^2)\\
\mathbb{P}(\gamma_{i,j\pm1}(k)=0) &= \mu \pm a\frac{\partial\mu}{\partial y}+\frac{1}{2}a^2\frac{\partial^2\mu}{\partial y^2}+o(a^2).
\end{aligned}
\tag{10}
$$

where again a represents the linear size of each site. Making use of the relation $\mu = 1-\rho-\phi$ and defining as usual

$$\lim_{a,\Delta t\to 0}\frac{\alpha a^2}{\Delta t}=D_\rho \qquad \lim_{a,\Delta t\to 0}\frac{\beta a^2}{\Delta t}=D_\phi,$$

we obtain

$$\frac{\partial\rho}{\partial t}=D_\rho((1-\phi)\nabla^2\rho+\rho\nabla^2\phi)$$

for the tagged species. Under the hypotesis of low concentration of the tagged agents, we finally get:

$$\frac{\partial\phi}{\partial t}=D_\phi\nabla^2\phi$$

for the evolution of the bulk density.

II. ON THE VALIDITY OF THE MEAN FIELD APPROXIMATION: COMPARING STOCHASTIC AND MEAN FIELD SIMULATIONS IN $2D$

To test the adequacy of the proposed mean field model we have performed a campaign of numerical simulations, with reference to the 2D setting. More specifically we have implemented a montecarlo scheme to solve the stochastic process under scrutiny and so trace the evolution of the tagged particle in time. At each time iteration, all crowders and the tagged particle can update their position, moving at random, and with equal probability, in one of the four allowed directions, provided the selected target site is unoccupied. If the site at destination is occupied, the move is rejected and the particles keep their original positions. The order of selection of the particles is, at each iteration, randomized. By averaging over many independent realizations, one can reconstruct the normalized histogram of the position visited by the crowders at a given time t and compare it with the density profile ρ obtained upon integration of the mean field system (7). To carry out the numerical integration of the above partial differential equations we assumed a forward difference approximation in time and replaced the spatial derivatives by centered approximations. The result of the comparison is reported in figures 1(a) and 1(b), for two choices of the initial conditions. In figure 1(a), the tagged particle is initially positioned in the middle of a two dimensional waterbag, filled with crowders, with average density equal to ϕ_0. In figure 1(a), the tagged particle is instead positioned, at time $t=0$, in the center of an empty region, a square of assigned size. The crowders are instead assumed to occupy an adjacent domain with average uniform density ϕ_0. In both cases, the agreement between stochastic and mean field simulations is satisfying.

III. ALTERNATIVE DERIVATION OF THE MODEL USING A COARSE GRAINED PICTURE

In this final section we discuss an alternative derivation of model (10), which assumes a coarse-grained decription of the scrutinized problem. The derivation follows a different philosphy: it is here carried out in one dimension, but readily generalizes to the relevant $d=3$ setting. We consider the physical space to be partitioned in Ω patches, also called *urns*. Each patch has a maximum carrying capacity - it can be filled with N particles at most. Labelling m_i the number of tagged particles contained in urn i, and with n_i the corresponding number of crowders, one can write:

$$n_i+m_i+v_i=N \quad \forall i$$

where v_i stands for the number of vacancies, the empty cases in patch i that can be eventually filled by incoming particles. The excluded-volume prescription is here implemented by requiring that particles can move only into the nearest-neighbor patches that exhibit vacancies,

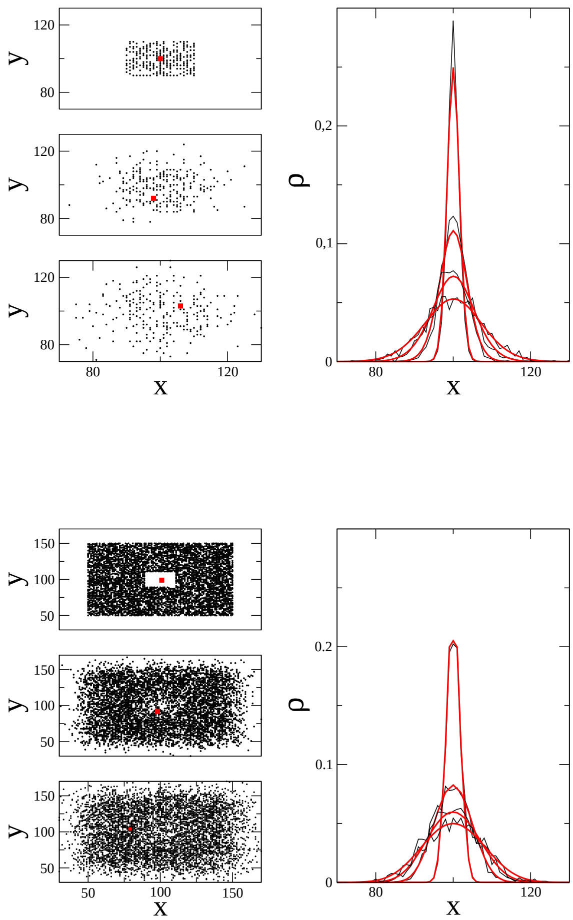

FIG. 1: Comparison between stochastic (thin solid lines) and mean field simulations (thick solid line). The stocastic simulations are averaged over 20000 realizations. Here $\phi_0 = 0.5$. Two dimensional snapshots of the stochastic simulations are also displayed. The crowders are plotted as small (black online) circles. The tagged particle is represented by the filled (red online) square. Upper panel: initial condition (see first snapshot, top left panel) originating a super-diffusive transient. Lower panel initial condition (see first snapshot, top left panel), causing a sub-diffusive transient.

as exemplified by the following chemical reactions

$$\begin{aligned} \mathcal{M}_i + V_j &\xrightarrow{\frac{\delta}{z\Omega}} \mathcal{M}_j + V_i \\ \mathcal{N}_i + V_j &\xrightarrow{\frac{\delta}{z\Omega}} \mathcal{N}_j + V_i \end{aligned} \tag{11}$$

Here z is the number of nearest-neighbor patches and $\mathcal{M}_i, \mathcal{N}_i, V_i$ are respectively a particle of type $\mathcal{M}$ (the tagged particles), of type $\mathcal{N}$ (the crowders) or a vacancy belonging to the i-patch.

This is stochastic process governed, under the Markov hypothesis, by a Master equation for the probability $P(\mathbf{n}, \mathbf{m}, t)$ of finding the system in a given state specified by the 2Ω dimensional vector $(\mathbf{n}, \mathbf{m}) = (n_1, ..., n_\Omega, m_1 ..., m_\Omega)$ at time t. The Master equation reads:

$$\begin{aligned} \frac{\partial P(\mathbf{n},\mathbf{m},t)}{\partial t} = \textstyle\sum_{n \neq n'} [T(\mathbf{n}, \mathbf{m}|\mathbf{n}', \mathbf{m}) P(\mathbf{n}', \mathbf{m}) + \\ T(\mathbf{n}, \mathbf{m}|\mathbf{n}, \mathbf{m}') P(\mathbf{n}, \mathbf{m}') - T(\mathbf{n}, \mathbf{m}'|\mathbf{n}, \mathbf{m}) P(\mathbf{n}, \mathbf{m}) - \\ T(\mathbf{n}', \mathbf{m}|\mathbf{n}, \mathbf{m}) P(\mathbf{n}, \mathbf{m})] \end{aligned} \tag{12}$$

where $T(\mathbf{a}|\mathbf{b})$ is the rate of transition from a state $\mathbf{a}$ to a compatible configuration $\mathbf{b}$. The allowed transitions are those that take place between neighboring patches as dictated by the chemical reactions (11). For example, the transition probability associated with the second of equations (11) reads

$$T(n_i - 1, n_j + 1|n_i, n_j) = \frac{\delta}{z\Omega} \frac{n_i}{N} \frac{v_j}{N} = \frac{\delta}{z\Omega} \frac{n_i}{N} (1 - \frac{n_j}{N} - \frac{m_j}{N}). \tag{13}$$

The transition rates bring into the equation an explicit dependence on the amount of molecules per patch N, the so-called system size. To proceed in the analysis, we make use of van Kampen system size expansion [**?**], which enables one to separate the site-dependent mean concentration $\phi_i(t)$ from the corresponding fluctuations ξ_i in the expression of the discrete number density of species $\mathcal{N}$. The fluctuations become less influent as the number of the agents is increased, an observation which translates in the following van Kampen ansatz:

$$\frac{n_i}{N}(t) = \phi_i(t) + \frac{\xi_i}{\sqrt{N}}. \tag{14}$$

In the following we will also assume just one tagged particle, the analysis extending straightforwardly to the case where a bunch of diluted particles is assumed to be dispersed in the background of crowders. Since the tagged particle belongs to one of the patches, it is convenient to look at the evolution of

$$P_k(\mathbf{n}, t) = P(\mathbf{n}, \underbrace{0, 0, ..., 0}_{k-1}, 1, \underbrace{0, ..., 0, 0}_{\Omega - k}, t)$$

in the master equation (12). $P_k(\mathbf{n}, t)$ is the probability that the target particle be in the k-patch, for a particular configuration $\mathbf{n}$ of species $\mathcal{N}$. The Master equation can be hence written in the following compact form

$$\frac{\partial P_k(\mathbf{n},t)}{\partial t} = \sum_{i=1}^{\Omega}\sum_{j\in i-1,i+1}(\epsilon_j^-\epsilon_i^+-1)T(n_i-1,n_j+1|n_i,n_j)P_k(n_i,n_j,t) + \sum_{i=1}^{\Omega}\left\{-\sum_{j\in i-1,i+1}\frac{\delta}{z\Omega}\frac{1}{N}\left(1-\frac{n_j}{N}\right)P_k + \sum_{j\in i-1,i+1}\frac{\delta}{z\Omega}\frac{1}{N}\left(1-\frac{n_k}{N}\right)P_j\right\} \tag{15}$$

where use has been made of the shift operators:

$$\epsilon_i^{\pm}f(....,n_i,.....) = f(....,n_i\pm 1,.....).$$

Under the van Kampen prescription [?], one can expand the transition rates in power of $1/\sqrt{N}$. For example,

$$T(n_i-1,n_j+1|n_i,n_j) = \frac{\delta}{z\Omega}\left\{(\phi_i(1-\phi_j)) + \frac{1}{\sqrt{N}}\left[\xi_i(1-\phi_j)-\xi_j\phi_i\right] + \frac{1}{N}\left[-\xi_i\xi_j - m_j\phi_i\right] + \frac{1}{N^{\frac{3}{2}}}\left[-m_j\xi_i\right]\right\}$$

and also express the shift operators in terms of differential operators:

$$(\epsilon_j^-\epsilon_i^+-1) = \frac{1}{\sqrt{N}}\left(\frac{\partial}{\partial\xi_i}-\frac{\partial}{\partial\xi_j}\right)+\frac{1}{2N}\left(\frac{\partial}{\partial\xi_i}-\frac{\partial}{\partial\xi_j}\right)^2+O(\frac{1}{N^{\frac{3}{2}}})$$

$$(\epsilon_j^-\epsilon_i^+-1)T(n_i-1,n_j+1|n_i,n_j)P(n_i,n_j,t) = \tfrac{1}{\sqrt{N}}\left[\left(\tfrac{\partial}{\partial\xi_i}-\tfrac{\partial}{\partial\xi_j}\right)\left(\tfrac{\delta}{z\Omega}(\phi_i(1-\phi_j))\Pi_k(\xi,t)\right)\right] + \tfrac{1}{N}\left[\left(\tfrac{\partial}{\partial\xi_i}-\tfrac{\partial}{\partial\xi_j}\right)\left(\tfrac{\delta}{z\Omega}(\xi_i(1-\phi_j)+\xi_j\phi_i)\Pi_k(\xi,t)\right) + \tfrac{1}{2}\left(\tfrac{\partial}{\partial\xi_i}-\tfrac{\partial}{\partial\xi_j}\right)^2\left(\tfrac{\delta}{z\Omega}(\phi_i(1-\phi_j))\Pi_k(\xi,t)\right)\right] + O\left(\tfrac{1}{N^{\frac{3}{2}}}\right).$$

Notice that m_i/N cannot be approximated as a continuum-like density, the continuum limit being not appropriate for the case of a single tracer.

We then define a new probability distribution $\Pi_k(\boldsymbol{\xi},\tau)$, function of the vector $\boldsymbol{\xi}$ and the scaled time $\tau = \frac{t}{N\Omega}$. In terms of the new probability distribution $\Pi_k(\boldsymbol{\xi},\tau)$ the left hand side of (15) becomes

$$\frac{\partial P_k}{\partial t} = -\frac{1}{\sqrt{N}\Omega}\sum_{i=1}^{\Omega}\frac{\partial\Pi_k}{\partial\xi_i}\dot{\phi}_i + \frac{1}{N\Omega}\frac{\partial\Pi_k}{\partial t}.$$

equation (13) takes the form

The leading order contribution in $(\frac{1}{\sqrt{N}})$ gives:

$$-\frac{1}{\Omega}\sum_{i=1}^{\Omega}\frac{\partial\Pi_k}{\partial\xi_i}\dot{\phi}_i = \frac{\delta}{z\Omega}\sum_{i=1}^{\Omega}\sum_{j\in\{i-1,i+1\}}\phi_i(1-\phi_j)\left(\frac{\partial\Pi_k}{\partial\xi_i}-\frac{\partial\Pi_k}{\partial\xi_j}\right) \tag{16}$$

which yields

$$\sum_{i=1}^{\Omega}\frac{\partial\Pi_k}{\partial\xi_i}\dot{\phi}_i = \frac{\delta}{z}\sum_{i=1}^{\Omega}-\frac{\partial\Pi_k}{\partial\xi_i}(2\phi_i-\phi_{i-1}-\phi_{i+1}) \tag{17}$$

and finally:

$$\dot{\phi}_i = \frac{\delta}{2}\Delta\phi_i \tag{18}$$

where Δ is the discrete Laplacian operator defined as $\Delta\phi_i = \frac{2}{z}\sum_{j\in i}(\phi_j-\phi_i)$, where $\sum_{j\in i}$ means a summation over the sites, j, which are nearest-neighbors of site i. By taking the size of the patches to zero, one recovers the standard diffusion equation for species ϕ, in agreement with the result reported in the main body of the paper. Consider now the following identities:

$$
\begin{aligned}
&\frac{\delta}{z}\sum_{i=1}^{\Omega}\sum_{j\in\{i-1,i+1\}}(\frac{\partial}{\partial\xi_i}-\frac{\partial}{\partial\xi_j})(\xi_i(1-\phi_j)-\xi_j\phi_i)\Pi_k \\
&=\frac{\delta}{z}\sum_{i=1}^{\Omega}(\frac{\partial}{\partial\xi_i}-\frac{\partial}{\partial\xi_{i-1}})(\xi_i(1-\phi_{i-1})-\xi_{i-1}\phi_i)\Pi_k+\frac{\delta}{z}\sum_{i=1}^{\Omega}(\frac{\partial}{\partial\xi_i}-\frac{\partial}{\partial\xi_{i+1}})(\xi_i(1-\phi_{i+1})-\xi_{i+1}\phi_i)\Pi_k \\
&=\frac{\delta}{z}\sum_{i=1}^{\Omega}\frac{\partial}{\partial\xi_i}\Big((\xi_i(1-\phi_{i-1})-\xi_{i-1}\phi_i)\Pi_k+(\xi_i(1-\phi_{i+1})-\xi_{i+1}\phi_i)\Pi_k\Big) \\
&-\frac{\delta}{z}\sum_{i=1}^{\Omega}\frac{\partial}{\partial\xi_i}(\xi_{i+1}(1-\phi_i)-\xi_i\phi_{i+1})\Pi_k-\frac{\delta}{z}\sum_{i=1}^{\Omega}\frac{\partial}{\partial\xi_i}(\xi_{i-1}(1-\phi_i)-\xi_i\phi_{i-1})\Pi_k \\
&=\frac{\delta}{2}\sum_{i=1}^{\Omega}-\Delta\xi_i\Pi_k
\end{aligned}
$$

and

$$
\begin{aligned}
&\frac{\delta}{z}\sum_{i=1}^{\Omega}\sum_{j\in\{i-1,i+1\}}\left(\frac{\partial}{\partial\xi_i}-\frac{\partial}{\partial\xi_j}\right)^2(\phi_i(1-\phi_j))\Pi_k \\
&=\frac{\delta}{z}\sum_{i=1}^{\Omega}\frac{\partial^2}{\partial\xi_i^2}\Big(\phi_i(1-\phi_{i-1})\Pi_k\Big)+\frac{\partial^2}{\partial\xi_i^2}\Big(\phi_i(1-\phi_{i+1})\Pi_k\Big)\frac{\partial^2}{\partial\xi_{i+1}^2}\Big(\phi_i(1-\phi_{i+1})\Pi_k\Big)+\frac{\partial^2}{\partial\xi_{i-1}^2}\Big(\phi_i(1-\phi_{i-1})\Pi_k\Big) \\
&-\frac{2\partial^2}{\partial\xi_i\partial\xi_{i-1}}\Big(\phi_i(1-\phi_{i-1})\Pi_k\Big)-\frac{2\partial^2}{\partial\xi_i\partial\xi_{i+1}}\Big(\phi_i(1-\phi_{i+1})\Pi_k\Big) \\
&=\frac{\delta}{z}\sum_{i=1}^{\Omega}\frac{\partial^2}{\delta\xi_i^2}(2\phi_i+\phi_{i-1}+\phi_{i+1}-2\phi_i(\phi_{i+1}+\phi_{i-1}))\Pi_k+\frac{\partial^2}{\partial\xi_i\partial\xi_{i-1}}\Big(-2\phi_i(1-\phi_{i-1})\Big)\Pi_k \\
&+\frac{\partial^2}{\partial\xi_i\partial\xi_{i+1}}\Big(-2\phi_i(1-\phi_{i+1})\Big)\Pi_k
\end{aligned}
$$

Making use of the above relations, at the next to next-to-leading corrections one eventually gets

$$
\begin{aligned}
\frac{\partial\Pi_k}{\partial t}&=\frac{\delta}{2}\sum_{i=1}^{\Omega}\frac{\partial}{\partial\xi_i}\Big(-\Delta\xi_i\Pi_k\Big)+\frac{\delta}{2z}\sum_{i=1}^{\Omega}\sum_{i=i-1}^{i+1}\frac{\partial}{\partial\xi_i}\frac{\partial}{\partial\xi_j}\Big(B_{i,j}\Pi_k\Big) \\
&+\frac{\delta}{z}\Big((1-\phi_k)\Pi_{k-1}-(2-\phi_{k+1}-\phi_{k-1})\Pi_k+(1-\phi_k)\Pi_{k+1}\Big)
\end{aligned}
$$

Here B represents the diffusion matrix, whose entries are

$$
\begin{aligned}
B_{i,i}&=2\phi_i+\phi_{i-1}+\phi_{i+1}-2\phi_i(\phi_{i+1}+\phi_{i-1}) \\
B_{i,i-1}&=(-2\phi_i(1-\phi_{i-1})) \\
B_{i,i+1}&=(-2\phi_i(1-\phi_{i+1})).
\end{aligned}
\tag{19}
$$

. To provide a mean-field description of the inspected problem, we consider the probability function of the tagged agent integrated over the fluctuations of the $\mathcal{N}$-particles. In formulae:

$$\rho_k(t) = \int \Pi_k d\boldsymbol{\xi}$$

whose evolution is governed by

$$\begin{aligned}\frac{\partial \rho_k}{\partial t} &= \frac{\delta}{z}\big((1-\phi_k)\rho_{k-1} - (2-\phi_{k+1}-\phi_{k-1})\rho_k \\ &+ (1-\phi_k)\rho_{k+1}\big) = \frac{\delta}{2}(\Delta\rho_k - \phi_k\Delta\rho_k + \rho_k\Delta\phi_k)\end{aligned}$$

The the last expression involves the discrete laplacian Δ defined above. In the continuum limit, and considering a straightforward generalization to higher dimensions, one gets

$$\frac{\partial \rho(\mathbf{r},t)}{\partial t} = D_\rho(1-\phi(\mathbf{r},t))\nabla^2\rho(\mathbf{r},t) + D_\rho\rho(\mathbf{r},t)\nabla^2\phi(\mathbf{r},t)$$

where D_ρ is the diffusion coefficient of the tagged particle. One can finally write the non-linear equation for ρ as a Fokker Plank equation:

$$\begin{aligned}\frac{\partial \rho(\mathbf{r},t)}{\partial t} &= \nabla^2\Big(D(1-\phi(\mathbf{r},t))\rho(\mathbf{r},t)\Big) \\ &+2D\nabla\Big(\rho(\mathbf{r},t)\nabla\phi(\mathbf{r},t)\Big)\end{aligned}$$

Hence, by neglecting the role of fluctuations, which amounts to operating in the mean-field limit, a nonlinear partial differential equation is found for the density of the tagged species, coupled to a standard diffusion equation for the background density:

$$\begin{cases}\frac{\partial \phi(\mathbf{r},t)}{\partial t} = D\nabla^2\phi(\mathbf{r},t) \\ \frac{\partial \rho(\mathbf{r},t)}{\partial t} = \nabla^2\Big(D(1-\phi(\mathbf{r},t))\rho(\mathbf{r},t)\Big) + 2D\nabla\Big(\rho(\mathbf{r},t)\nabla\phi(\mathbf{r},t)\Big)\end{cases} \tag{20}$$

This system constitutes the generalization of model (10) to higher dimensions. It is worth emphasising that the second of eqs. (20) can be also cast in the alternative form:

$$\frac{\partial \rho(\mathbf{r},t)}{\partial t} = \nabla\cdot\left(D\left(1-\phi(\mathbf{r},t)\right)\nabla\rho(\mathbf{r},t) + D\rho(\mathbf{r},t)\nabla\phi(\mathbf{r},t)\right)$$