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DERIVATION OF A KINETIC MODEL FROM A STOCHASTIC PARTICLE SYSTEM

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Abstract. We study a stochastic lattice particle system with exclusion principle. A kinetic equation and its diffusion limit are formally derived from the Monte Carlo dynamics. This derivation is investigated analytically and numerically and compared with the classical hydrodynamic limit of the stochastic exclusion process. Numerical results are presented for different values of jump probabilities.

1. **Introduction.** Interactions of particles are primarily motivated by a variety of applications in materials science, physics and stochastics. There exists a huge amount of literature offering different mathematical approaches. On the one hand, microscopic models like stochastic particle systems and related Monte Carlo methods provide a fine-scale description of particle jump processes, for an overview see [6, 13, 2, 5, 7, 10]. On the other hand, coarse scale or macroscopic models are based on partial differential equations for averaged quantities instead of individual particles [2, 12, 14, 15]. On an intermediate scale the particle system can be described by Boltzmann-like kinetic equations. In the following, starting from a stochastic particle system, we derive a kinetic model and associated hydrodynamic limits. We show that under certain assumptions a discrete kinetic model and a related diffusion equation can be derived.

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We consider a stochastic particle system with an exclusion principle in a one-dimensional situation, see for example [6, 13, 16]. Suppose atoms are restricted to a periodic 1-d lattice. The spatial grid is denoted by $y_i = -L+(i-1)\Delta y$, $i = 1, \dots, M$ where the lattice spacing is $\Delta y = 2L/(M-1)$ and L is a positive constant describing the (left and right) boundary of the grid. The time step between the jumps is given by Δt with $t_n = n\Delta t$, $n \in N$. Atoms are supposed to jump only to the left or right neighbouring site, i.e., we do not consider long jumps. Due to the exclusion principle only one atom is considered at a special grid point. To determine the probability of a jump one has to consider the relevant neighbours. Here we restrict to nearest neighbour interactions. Thus, if the atom under consideration is at the point y_i and jumps to the point y_{i+1}, then one has to consider additionally the atoms at the positions y_{i-1}, y_{i+2}. We denote by P the probability of a jump. Denoting a site with an atom by 1 and an empty site by 0, the following cases have to be distinguished:

y_{i-1}	y_i	y_{i+1}	y_{i+2}	
1	1	0	1	$P = \alpha_1$
0	1	0	0	$P = \alpha_2$
1	1	0	0	$P = \alpha_3$
0	1	0	1	$P = \alpha_4$

with probabilities $\alpha_1, \alpha_2, \alpha_3, \alpha_4 \in [0, 1]$. We assume that the gradient condition [13] for a one-dimensional exclusion process is fulfilled:

$$\alpha_1 + \alpha_2 = \alpha_3 + \alpha_4 \tag{1}$$

and introduce furthermore the relation

$$e = \frac{\alpha_4}{\alpha_3} \in [0, \infty).$$

Here, the factor $e > 1$ describes attractive potentials and $e < 1$ repulsive ones. Without restricting generality one may divide all α_i by α_2 and rename the hopping rates:

$$\alpha_1' = 1 + \alpha + \beta, \quad \alpha_2' = 1, \quad \alpha_3' = 1 + \alpha, \quad \alpha_4' = 1 + \beta,$$

where $\alpha_1', \alpha_3', \alpha_4' \in [0, \infty)$. This choice of parameters is admissible since the gradient condition (1) is again satisfied. In our considerations, in particular, we stick to the special situation

$$e = \frac{1+\beta}{1+\alpha} \stackrel{!}{=} 1,$$

i.e. a balance between repulsion and attraction. This obviously implies that $\alpha = \beta$. From this it follows that the remaining rates have to be set in the following way:

$$\alpha_1' = 1 + 2\alpha, \quad \alpha_2' = 1, \quad \alpha_3' = 1 + \alpha = \alpha_4'.$$

This parameter setting will be starting point for our further investigations. We refer to [13] for a detailed investigation using stochastic analysis in this case. The more general case has been treated in [6]. Explicit computations can be found in the work of Zwerger [16].

In the next section we state a kinetic approximation for the above stochastic process. For the special case $\alpha = \beta$ it is shown in section 3 that this kinetic equation can be derived from the stochastic particle system under a molecular chaos assumption for the two particle distribution. However, for the general case this can not be valid due to the difference in the hydrodynamic limit of the kinetic equation and the stochastic particle system. Numerical comparisons of a Monte Carlo method, the kinetic equation and the diffusion equation are presented in section 5 using numerical methods discussed in section 4.

2. **The Kinetic Equation.** We assume that the probabilities for a certain configuration can be determined from the one-particle probability density. To set up a kinetic equation we consider the probabilities that a particle jumps from position y_i to another position (Loss) and the probabilities that a particle jumps to position y_i (Gain) assuming that this position is initially empty. We denote by $f_i = f_i(t)$ the probability of having a particle at y_i at time t, $f_i \in [0,1]$. The complementary probability is then given by $\overline{f}_i = 1 - f_i$. We use f_i^n as a notation for the probability of having a particle at y_i at time t_n and assume independence of the probabilities. An evolution equation is formally given by collecting the gain and loss terms for the distribution function at y_i:

$$\partial_t f_i = G(f) - L(f) \tag{2}$$

with gain terms

$$\begin{aligned} G(f) = \; & \overline{f}_i \Big(\alpha_1 [f_{i-1} f_{i+1} f_{i+2} + f_{i-2} f_{i-1} f_{i+1}] \\ & +\alpha_2 [\overline{f}_{i-1} f_{i+1} \overline{f}_{i+2} + \overline{f}_{i-2} f_{i-1} \overline{f}_{i+1}] \\ & +\alpha_3 [\overline{f}_{i-1} f_{i+1} f_{i+2} + f_{i-2} f_{i-1} \overline{f}_{i+1}] \\ & +\alpha_4 [f_{i-1} f_{i+1} \overline{f}_{i+2} + \overline{f}_{i-2} f_{i-1} f_{i+1}] \Big) \end{aligned}$$

and loss terms

$$\begin{aligned} L(f) = \; & f_i \Big(\alpha_1 [f_{i-1} \overline{f}_{i+1} f_{i+2} + f_{i-2} \overline{f}_{i-1} f_{i+1}] \\ & +\alpha_2 [\overline{f}_{i-1} \overline{f}_{i+1} \overline{f}_{i+2} + \overline{f}_{i-2} \overline{f}_{i-1} \overline{f}_{i+1}] \\ & +\alpha_3 [f_{i-1} \overline{f}_{i+1} \overline{f}_{i+2} + \overline{f}_{i-2} \overline{f}_{i-1} f_{i+1}] \\ & +\alpha_4 [f_{i-2} \overline{f}_{i-1} \overline{f}_{i+1} + \overline{f}_{i-1} \overline{f}_{i+1} f_{i+2}] \Big). \end{aligned}$$

The time discrete version of this system is apparently given by

$$f_i^{n+1} - f_i^n = \Delta t \left(G(f^n) - L(f^n) \right). \tag{3}$$

Note that after rescaling time in (2) with α_2 we obtain the same equation with the values α_i' instead of α_i in the above expressions for the gain and loss terms.

Although a stability result for the kinetic equation can be proven for the whole range of parameters, see subsection 4.1, it will turn out that, in general, the kinetic equation is not a valid approximation of the stochastic particle system. This is only true for the special case mentioned above, which can be seen as follows. To derive a partial differential equation (cf. [3]) from the above kinetic we consider a diffusive scaling and multiply the probabilities by $1/(\Delta y)^2$ considering the equation

$$\partial_t f_i = \frac{1}{(\Delta y)^2} \Big[G(f) - L(f) \Big]. \tag{4}$$

Using the commercial software package MAPLE [11] a Taylor expansion of the above expressions with respect to Δy is carried out. Obviously the terms to order $\mathcal{O}(\frac{1}{\Delta y^2})$ on the right hand side cancel as well as the terms to order $\mathcal{O}(\frac{1}{\Delta y})$. Only terms of order $\mathcal{O}(1)$ remain and we obtain a diffusion equation:

$$\partial_t f = (d(f) f')' \tag{5}$$

with nonlinear diffusion coefficient

$$d(f) = 3(\beta - \alpha) f^2 + 2(2\alpha - \beta) f + 1. \tag{6}$$

However, the limit of the stochastic particle system is given by another diffusion coefficient known as the Green Kubo formula, see [6, 13, 16]:

$$d_{GK}(f) = \frac{(1 - y(f))}{2\chi(f)} \Big[2 + \alpha + \beta + (\alpha - \beta) y(f) + (\alpha + \beta) \sigma(f) (1 - y(f)) \Big]$$

where

$$\sigma(x) = 2x - 1, \quad \chi(x) := \sqrt{\sigma^2(x) + (1 - \sigma^2(x))e}, \quad y(x) := \frac{\chi(x) - 1}{\chi(x) + 1}.$$

Note that in general this will not be equal to the above expression for the diffusion coefficient (6). We consider two special cases, see [6]:

Case 1: We set $\alpha = -\beta$, and therefore

$$\alpha_1' = \alpha_2' = 1, \quad \alpha_3' = 1 + \alpha, \quad \alpha_4' = 1 - \alpha.$$

Then, the diffusion coefficient in (6) reduces to

$$d(f) = 1 + 6\alpha f(1 - f)$$

and the Green-Kubo can be rewritten as

$$d_{GK}(f) = \frac{2(\chi(f)(1 + \alpha) + 1 - \alpha)}{(1 + \chi(f))^2 \chi(f)}.$$

In this case the two expressions do not coincide, see section 5 for a numerical experiment. Obviously, for $e > 5$, or $\alpha < -2/3$, i.e. for strongly attractive potentials, the expression for $d(f)$ becomes even negative.

Case 2: This is the special situation mentioned at the end of the last section with $e = 1$, i.e. $\alpha = \beta$. In this case we have

$$\alpha_1' = 1 + 2\alpha, \quad \alpha_2' = 1, \quad \alpha_3' = 1 + \alpha = \alpha_4'$$

and the condensed kinetic equation

$$\partial_t f_i = G(f) - L(f)$$

with

$$G(f) = \overline{f}_i \Big(f_{i-1} + f_{i+1} + \alpha [f_{i+1} f_{i+2} + f_{i-1} f_{i-2} + 2 f_{i-1} f_{i+1}] \Big)$$

and

$$L(f) = f_i \Big(f_{i-1} + f_{i+1} + \alpha [f_{i-1} \overline{f}_{i+1} + \overline{f}_{i-1} f_{i+1} + \overline{f}_{i-1} f_{i-2} + \overline{f}_{i+1} f_{i+2}] \Big).$$

Moreover, a small computation shows that the expression reduces to

$$\begin{aligned} \partial_t f_i = {} & f_{i+1} - 2 f_i + f_{i-1} \\ & + \alpha \Big(f_{i+1} f_{i+2} + f_{i-1} f_{i-2} + 2 f_{i-1} f_{i+1} \\ & - f_i f_{i-1} - f_i f_{i+1} - f_i f_{i-2} - f_i f_{i+2} \Big). \end{aligned} \tag{7}$$

The corresponding partial differential equation is

$$\partial_t f = (d(f) f')'$$

with the linear diffusion coefficient

$$d(f) = 2\alpha f + 1.$$

This result coincides with the one obtained by the Green-Kubo formula, see [13]. In this case a rigorous derivation of the kinetic equation from the stochastic particle system might be possible. The asymptotic validity of the kinetic equation for $\alpha = \beta$, i.e. in case of a balance between repulsion and attraction, is formally investigated in the next section starting from the stochastic particle system.

3. **The Liouville / master equation for the microscopic system.** This chapter is devoted to the derivation of equation (7). As before we consider M sites on a periodic lattice and N indiscernable particles. Let x_1 be the site of the first particle, x_i the site of the ith particle. Since there is an exclusion principle for the sites we consider the configuration space.

$$\Delta^N = \{(x_1, \cdots, x_N) \in \{1, \cdots M\}^N, |\forall i, j,\, i \neq j : x_i \neq x_j\}.$$

Define the set of particles having a direct left / right neighbour

$$\Delta^{\pm}_{x,j} = \{(x_1, \cdots, x_N) \in \{1, \cdots M\}^N, x_j = x,\, \exists\, i \neq j \,\text{such that}\; x_i = x \pm 1\}$$

and the set of particles with a neighbour on the site next to the directly neighbouring site

$$\Delta^{\pm,2}_{x,j} = \{(x_1, \cdots, x_N) \in \{1, \cdots M\}^N, x_j = x,\, \exists\, i \neq j \,\text{such that}\; x_i = x \pm 2\}.$$

Let $F^N(x_1, \cdots, x_j, \cdots, x_N)$ denote the N-particle probability distribution. Then, the N-particle evolution equation is

$$\begin{aligned}
\partial_t F^N \;=\;& \sum_{j=1}^{N} \Big[\Big(1 - \chi(\Delta^-_{x_j+1,j})\Big) \Big(1 + \alpha \Big(\chi(\Delta^{-,2}_{x_j+1,j}) + \chi(\Delta^+_{x_j+1,j})\Big)\Big) \Big] \\
& F^N(x_1, \cdots, x_j + 1, \cdots, x_N) \\
+\;& \sum_{j=1}^{N} \Big[\Big(1 - \chi(\Delta^+_{x_j-1,j})\Big) \Big(1 + \alpha \Big(\chi(\Delta^-_{x_j-1,j}) + \chi(\Delta^{+,2}_{x_j-1,j})\Big)\Big) \Big] \\
& F^N(x_1, \cdots, x_j - 1, \cdots, x_N) \\
-\;& \sum_{j=1}^{N} \Big[\Big(1 - \chi(\Delta^-_{x_j,j})\Big) \Big(1 + \alpha \Big(\chi(\Delta^{-,2}_{x_j,j}) + \chi(\Delta^+_{x_j,j})\Big)\Big) \\
& + \Big(1 - \chi(\Delta^+_{x_j,j})\Big) \Big(1 + \alpha \Big(\chi(\Delta^-_{x_j,j}) + \chi(\Delta^{+,2}_{x_j,j})\Big)\Big) \Big] F^N(x_1, \cdots, x_N).
\end{aligned}$$

We consider the d-particle probability distribution

$$F^d(x_1, \cdots, x_d) = \sum_{x_{d+1}, \cdots, x_N} F^N(x_1, \cdots, x_N)$$

and the number density function denoting the number of particles at $x_1, \cdots, x_d$:

$$f^d(x_1, \cdots, x_d) = \frac{N!}{(N-d)!} F^d(x_1, \cdots, x_d).$$

In the following we determine an equation for the 1-particle distribution function f^1 by integrating the evolution equation over $x_2, \cdots, x_N$. We treat the terms in the above equation separately:

First, integration of the terms involving only the $1-$particle distribution function yields

$$f^1(x_1 - 1) - 2f^1(x_1) + f^1(x_1 + 1).$$

The linear terms involving $\chi(\Delta^+_{x_j,j})$, $\chi(\Delta^-_{x_j,j})$, etc. are treated as follows. We investigate terms which evaluate the distribution functions for the nearest neighbour regions, namely $\Delta^{\pm}_{x,j}$ and $\Delta^{\pm,2}_{x,j}$.

First of all we consider the term

$$(1-\alpha)\sum_{j=1}^{N}\sum_{x_2,\cdots,x_N}\chi(\Delta^{+}_{x_j,j}))F^N(x_1,\cdots,x_N). \tag{8}$$

Define for $j\neq 1$ the set of particles having a neighbour equal to the first particle

$$\Delta^{\pm}_{x_j,j,1}=\{(x_1,\cdots,x_N)\in\{1,\cdots M\}^N,|x_1=x_j\pm 1\}$$

and the set of particles having a neighbour not equal to the first particle

$$\overline{\Delta^{\pm}_{x_j,j,1}}=\{(x_1,\cdots,x_N)\in\{1,\cdots M\}^N,|\text{there is } i\neq 1: x_i=x_j\pm 1\}.$$

Then, we define the union of both sets as

$$\Delta^{\pm}_{x_j,j}=\Delta^{\pm}_{x_j,j,1}\cup\overline{\Delta^{\pm}_{x_j,j,1}}.$$

This implies that the sum above is equal to

$$\begin{aligned}(1-\alpha)\sum_{j\neq 1}\sum_{x_2,\cdots,x_N}&\left(\chi(\Delta^{+}_{x_j,j,1})+\chi(\overline{\Delta^{+}_{x_j,j,1}})\right)F^N(x_1,\cdots,x_N)\\&+\sum_{x_2,\cdots,x_N}\chi(\Delta^{+}_{x_1,1})F^N(x_1,\cdots,x_N).\end{aligned}$$

After permutation we end up with an expression where only the 2−particle and the 3−particle distribution are relevant:

$$\begin{aligned}&(1-\alpha)(N-1)\sum_{x_2,\cdots,x_N}\left(\chi(\Delta^{+}_{x_2,2,1})+\chi(\overline{\Delta^{+}_{x_2,2,1}})\right)F^N(x_1,\cdots,x_N)\\&\qquad+\sum_{x_2,\cdots,x_N}\chi(\Delta^{+}_{x_1,1})F^N(x_1,\cdots,x_N)\\&=(1-\alpha)(N-1)\left[F^2(x_1,x_1-1)+\sum_{x_2\neq x_1,x_2\neq x_1-1}(N-2)F^3(x_1,x_2,x_2+1)\right]\\&\qquad+(N-1)F^2(x_1,x_1+1).\end{aligned}$$

Going back to a normalized version, we obtain the terms:

$$\begin{aligned}&(1-\alpha)(N-1)\Big[\frac{1}{N(N-1)}f^2(x_1,x_1-1)\\&+\frac{1}{N(N-1)(N-2)}\sum_{x_2\neq x_1,x_2\neq x_1-1}(N-2)f^3(x_1,x_2,x_2+1)\Big]\\&+\frac{1}{N(N-1)}(N-1)f^2(x_1,x_1+1),\end{aligned}$$

or, alternatively in a more condensed form,

$$(1-\alpha)\frac{1}{N}\Big[f^2(x_1,x_1-1)+\sum_{x_2\neq x_1,x_2\neq x_1-1}f^3(x_1,x_2,x_2+1)+f^2(x_1,x_1+1)\Big].$$

Now, in a further step, we consider the term

$$(1-\alpha)\sum_{j=1}^{N}\sum_{x_2,\cdots,x_N}\chi(\Delta^{-}_{x_j,j})F^N(x_1,\cdots,x_N). \tag{9}$$

In the same way as above one obtains

$$(1-\alpha)\frac{1}{N}\Big[f^2(x_1,x_1+1)+f^2(x_1,x_1-1)+\sum_{x_2\neq x_1,x_2\neq x_1+1} f^3(x_1,x_2,x_2-1)\Big].$$

Similarly, for the term

$$-\sum_{j=1}^{N}\sum_{x_2,\cdots,x_N}\chi(\Delta^-_{x_j+1,j})F^N(x_1,\cdots,x_j+1,\cdots,x_N) \tag{10}$$

we get

$$-\frac{1}{N}\Big[f^2(x_1,x_1+1)+f^2(x_1+1,x_1)+\sum_{x_2\neq x_1,x_2\neq x_1-1} f^3(x_1,x_2+1,x_2)\Big].$$

Next, we obtain that

$$\alpha\sum_{j=1}^{N}\sum_{x_2,\cdots,x_N}\chi(\Delta^+_{x_j+1,j})F^N(x_1,\cdots,x_j+1,\cdots,x_N) \tag{11}$$

is equal to

$$\alpha\frac{1}{N}\Big[f^2(x_1,x_1-1)+f^2(x_1+1,x_1+2)+\sum_{x_2\neq x_1-1,x_2\neq x_1-2} f^3(x_1,x_2+1,x_2+2)\Big].$$

The term

$$\alpha\sum_{j=1}^{N}\sum_{x_2,\cdots,x_N}\chi(\Delta^-_{x_j-1,j})F^N(x_1,\cdots,x_j-1,\cdots,x_N) \tag{12}$$

can be expressed as

$$\alpha\frac{1}{N}\Big[f^2(x_1,x_1+1)+f^2(x_1-1,x_1-2)+\sum_{x_2\neq x_1+1,x_2\neq x_1+2} f^3(x_1,x_2-1,x_2-2)\Big].$$

The term

$$-\sum_{j=1}^{N}\sum_{x_2,\cdots,x_N}\chi(\Delta^+_{x_j-1,j})F^N(x_1,\cdots,x_j-1,\cdots,x_N) \tag{13}$$

is equal to

$$-\frac{1}{N}\Big[f^2(x_1,x_1-1)+f^2(x_1-1,x_1)+\sum_{x_2\neq x_1,x_2\neq x_1+1} f^3(x_1,x_2-1,x_2)\Big].$$

$$\alpha\sum_{j=1}^{N}\sum_{x_2,\cdots,x_N}\chi(\Delta^{-,2}_{x_j+1,j})F^N(x_1,\cdots,x_j+1,\cdots,x_N) \tag{14}$$

gives

$$\alpha\frac{1}{N}\Big[f^2(x_1,x_1+2)+f^2(x_1+1,x_1-1)+\sum_{x_2\neq x_1-1,x_2\neq x_1+1} f^3(x_1,x_2+1,x_2-1)\Big].$$

Straightforwardly, we figure out that

$$\alpha\sum_{j=1}^{N}\sum_{x_2,\cdots,x_N}\chi(\Delta^{+,2}_{x_j-1,j})F^N(x_1,\cdots,x_j-1,\cdots,x_N) \tag{15}$$

is equal to

$$\alpha\frac{1}{N}\Big[f^2(x_1,x_1-2)+f^2(x_1-1,x_1+1)+\sum_{x_2\neq x_1+1,x_2\neq x_1-1}f^3(x_1,x_2-1,x_2+1)\Big]$$

and

$$-\alpha\sum_{j=1}^{N}\sum_{x_2,\cdots,x_N}\chi(\Delta^{-,2}_{x_j,j})F^N(x_1,\cdots,x_j,\cdots,x_N) \tag{16}$$

is equal to

$$-\alpha\frac{1}{N}\Big[f^2(x_1,x_1+2)+f^2(x_1,x_1-2)+\sum_{x_2\neq x_1,x_2\neq x_1+2}f^3(x_1,x_2,x_2-2)\Big].$$

Finally, one proves that

$$-\alpha\sum_{j=1}^{N}\sum_{x_2,\cdots,x_N}\chi(\Delta^{+,2}_{x_j,j})F^N(x_1,\cdots,x_j,\cdots,x_N) \tag{17}$$

is the same as

$$-\alpha\frac{1}{N}\Big[f^2(x_1,x_1-2)+f^2(x_1,x_1+2)+\sum_{x_2\neq x_1,x_2\neq x_1-2}f^3(x_1,x_2,x_2+2)\Big].$$

After permutations one observes that all terms involving f^3 in the rewritten forms of (8)– (17) are cancelled out. Further considerations of terms like

$$\sum_{j=1}^{N}\sum_{x_2,\cdots,x_N}\chi(\Delta^{+}_{x_j,j})\chi(\Delta^{-}_{x_j,j})F^N(x_1,\cdots,x_j,\cdots,x_N)$$

including $3-$particle correlations yield results depending only on f^3 and f^4. The permuation principle implicate that all these terms vanish again.

Alltogether, the f^1-evolution equation is given by

$$\begin{aligned}\frac{1}{N}\partial_t f^1(x_1)&=f^1(x_1-1)-2f^1(x_1)+f^1(x_1+1)\\ +\frac{\alpha}{N}\Big[f^2(x_1+1,x_1+2)&+f^2(x_1-1,x_1-2)+2f^2(x_1-1,x_1+1)\\ -f^2(x_1,x_1-1)-f^2(x_1,x_1+1)&-f^2(x_1,x_1-2)-f^2(x_1,x_1+2)\Big].\end{aligned}$$

Now, we rescale time with $\frac{1}{N}$ and define the density of particles as

$$n(x_i)=\frac{1}{M}f^1(x_i)$$

with $\sum_{i=1}^{M}n(x_i)=N/M$. Then, if a chaos assumption for the two particle distribution, i.e. $f^2(x_1,x_2)=f^1(x_1)f^1(x_2)$ is valid we obtain a closed equation for the density n:

$$\begin{aligned}\partial_t n(x_1)&=n(x_1-1)-2n(x_1)+n(x_1+1)\\ +\frac{\alpha M}{N}\Big[n(x_1+1)n(x_1+2)&+n(x_1-1)n(x_1-2)+2n(x_1-1)n(x_1+1)\\ -n(x_1)n(x_1-1)-n(x_1)n(x_1+1)&-n(x_1)n(x_1-2)-n(x_1)(x_1+2)\Big].\end{aligned}$$

In the limit $M, N \to \infty$ with $\frac{N}{M} \to 1$ we have $n(x_1) \to f_i$ with f_i being the probability for a particle at the lattice point $y_i = -L + (x_1 - 1)\Delta y$. Here f_i is given by the equation

$$\begin{aligned}
&\partial_t f_i = f_{i+1} - 2f_i + f_{i-1} \\
&+\alpha\Big(f_{i+1}f_{i+2} + f_{i-1}f_{i-2} + 2f_{i-1}f_{i+1} \\
&-f_i f_{i-1} - f_i f_{i+1} - f_i f_{i-2} - f_i f_{i+2}\Big)
\end{aligned}$$

This is in fact the kinetic equation stated in (7) for the special case $\alpha = \beta$.

Remark 1. *In the general case, i.e. α not equal to β, a derivation similiar to the above procedure can not be valid, since the resulting diffusion equation is not equal to the Green-Kubo formula.*

4. **Numerical methods.** In this section we discuss the numerical methods for the different levels of description, i.e. microscopic, kinetic and macroscopic level. See [9, 15] for related problems. On the microscopic level, that means the particle level, a stochastic Monte Carlo code has been implemented. For the kinetic level the discrete equation is used. For the diffusion equations we use a straightforward Finite-Difference scheme. In this section, we study some numerical properties of the kinetic equation and of the discretization scheme for the diffusion equation.

4.1. **Numerics for the kinetic equation.** On the kinetic level, the time and space discrete equation (3) is implemented. We investigate this equation analytically and prove a stability result using that the probabilities fulfill

$$0 \leq \alpha_i \leq 1.$$

The kinetic equation is rewritten as

$$f_i^{n+1} = f_i^n \left(1 - \frac{\Delta t}{(\Delta x)^2} A(i,n)\right) + \overline{f}_i \frac{\Delta t}{(\Delta x)^2} B(i,n) \tag{18}$$

with

$$\begin{aligned}
A(i,n) = \quad & \alpha_1[f_{i-1}\overline{f}_{i+1}f_{i+2} + f_{i-2}\overline{f}_{i-1}f_{i+1}] \\
&+\alpha_2[\overline{f}_{i-1}\overline{f}_{i+1}\overline{f}_{i+2} + \overline{f}_{i-2}\overline{f}_{i-1}\overline{f}_{i+1}] \\
&+\alpha_3[f_{i-1}\overline{f}_{i+1}\overline{f}_{i+2} + \overline{f}_{i-2}\overline{f}_{i-1}f_{i+1}] \\
&+\alpha_4[f_{i-2}\overline{f}_{i-1}\overline{f}_{i+1} + \overline{f}_{i-1}\overline{f}_{i+1}f_{i+2}]
\end{aligned}$$

and

$$\begin{aligned}
B(i,n) = \quad & \alpha_1[f_{i-1}f_{i+1}f_{i+2} + f_{i-2}f_{i-1}f_{i+1}] \\
&+\alpha_2[\overline{f}_{i-1}f_{i+1}\overline{f}_{i+2} + \overline{f}_{i-2}f_{i-1}\overline{f}_{i+1}] \\
&+\alpha_3[\overline{f}_{i-1}f_{i+1}f_{i+2} + f_{i-2}f_{i-1}\overline{f}_{i+1}] \\
&+\alpha_4[f_{i-1}f_{i+1}\overline{f}_{i+2} + \overline{f}_{i-2}f_{i-1}f_{i+1}]
\end{aligned}$$

by writing more shortly f_i instead of f_i^n. We prove

Lemma 4.1. *Let $0 \leq f_i^n \leq 1$ for all $i \in M$ and $0 \leq \frac{\Delta t}{(\Delta x)^2} A(i,n) \leq 1$ and $0 \leq \frac{\Delta t}{(\Delta x)^2} B(i,n) \leq 1$, then*

$$0 \leq f_i^{n+1} \leq 1, \quad \textit{for all } i \in M.$$

Proof. Define

$$a(i,n) = 1 - \frac{\Delta t}{(\Delta x)^2} A(i,n),$$
$$b(i,n) = \frac{\Delta t}{(\Delta x)^2} B(i,n).$$

Then

$$0 \le a(i,n), b(i,n) \le 1$$

and

$$f_i^{n+1} = f_i^n a(i,n) + \overline{f}_i^n b(i,n) \le f_i^n + \overline{f}_i^n = 1.$$

Moreover, obviously $0 \le f_i^{n+1}$, since all terms in the above expression for f_i^{n+1} are positive. □

We can now prove the following maximum principle.

Theorem 4.2. *Let the parabolic CFL condition*

$$2\frac{\Delta t}{(\Delta x)^2} \le 1$$

be fulfilled. Then, if $0 \le f_i^n \le 1$, *one has the condition that*

$$0 \le f_i^{n+1} \le 1, \quad \text{for all } i \in M.$$

Proof. According to Lemma 4.1 we have to prove that $0 \le A(i,n), B(i,n) \le 2$, if $0 \le f_i^n \le 1$. Both expressions are obviously positive. We have

$$\begin{aligned} A(i,n) &= \left(\alpha_1 f_{i+2} + \alpha_3 \overline{f}_{i+2}\right) f_{i-1}\overline{f}_{i+1} \\ &\quad + \left(\alpha_1 f_{i-2} + \alpha_3 \overline{f}_{i-2}\right) \overline{f}_{i-1} f_{i+1} \\ &\quad + \alpha_2 \left(\overline{f}_{i-1}\overline{f}_{i+1}\overline{f}_{i+2} + \overline{f}_{i-2}\overline{f}_{i-1}\overline{f}_{i+1}\right) \\ &\quad + \alpha_4 \left(f_{i-2}\overline{f}_{i-1}\overline{f}_{i+1} + \overline{f}_{i-1}\overline{f}_{i+1} f_{i+2}\right) \\ &\le f_{i-1}\overline{f}_{i+1} + \overline{f}_{i-1} f_{i+1} + f_{i-2}\overline{f}_{i-1}\overline{f}_{i+1} \\ &\quad + \overline{f}_{i-1}\overline{f}_{i+1} f_{i+2} + \overline{f}_{i-2}\overline{f}_{i-1}\overline{f}_{i+1} + \overline{f}_{i-1}\overline{f}_{i+1}\overline{f}_{i+2}, \end{aligned}$$

since

$$0 \le ac + b(1-c) \le 1$$

if $0 \le a, b, c \le 1$. This is equal to

$$\begin{aligned} & f_{i-1}\overline{f}_{i+1} + \overline{f}_{i-1} f_{i+1} + \overline{f}_{i-1}\overline{f}_{i+1} + \overline{f}_{i-1}\overline{f}_{i+1} \\ = \; & \overline{f}_{i+1}(f_{i-1} + \overline{f}_{i-1}) + \overline{f}_{i-1}(\overline{f}_{i+1} + f_{i+1}) = \overline{f}_{i+1} + \overline{f}_{i-1} \le 2. \end{aligned}$$

The same arguments give

$$\begin{aligned} B(i,n) &= \left(\alpha_1 f_{i-1} + \alpha_3 \overline{f}_{i-1}\right) f_{i+1} f_{i+2} \\ &\quad + \left(\alpha_1 f_{i+1} + \alpha_3 \overline{f}_{i+1}\right) f_{i-1} f_{i-2} \\ &\quad + \alpha_2 \left(\overline{f}_{i-1} f_{i+1}\overline{f}_{i+2} + \overline{f}_{i-2} f_{i-1}\overline{f}_{i+1}\right) \\ &\quad + \alpha_4 \left(f_{i-1} f_{i+1}\overline{f}_{i+2} + f_{i-1} f_{i+1}\overline{f}_{i-2}\right) \\ &\le \overline{f}_{i-1} f_{i+1}\overline{f}_{i+2} + \overline{f}_{i-2} f_{i-1}\overline{f}_{i+1} + f_{i+1} f_{i+2} \\ &\quad + f_{i-1} f_{i-2} + f_{i-1} f_{i+1}\overline{f}_{i+2} + f_{i-1} f_{i+1}\overline{f}_{i-2}. \end{aligned}$$

This is equal to

$$\begin{aligned} & \overline{f}_{i-1} f_{i+1}\overline{f}_{i+2} + f_{i-1} f_{i+1}\overline{f}_{i+2} + \overline{f}_{i-2} f_{i-1}\overline{f}_{i+1} \\ & + f_{i-1} f_{i+1}\overline{f}_{i-2} + f_{i+1} f_{i+2} + f_{i-1} f_{i-2} \\ = \; & f_{i+1}\overline{f}_{i+2} + f_{i-1}\overline{f}_{i-2} + f_{i+1} f_{i+2} + f_{i-1} f_{i-2} \\ = \; & f_{i+1} + f_{i-1} \le 2. \end{aligned}$$

□

4.2. **A numerical scheme for the macroscopic equation.** As proven in the last subsection a maximum principle is valid for the kinetic equation (3). A suitable numerical method for the diffusion equation (5) with the Green Kubo diffusion coefficient is a scheme where the diffusion coefficient $d(f)$ is treated in the following way:

$$\partial_t f_i = \frac{1}{(\Delta y)^2}[m_{i+1}(f_{i+1} - f_i) - m_i(f_i - f_{i-1})], \tag{19}$$

where $m_i = \frac{d(f_i)+d(f_{i-1})}{2}$.

We set $d(f) = d(0) \geq 0$ for $f \leq 0$ and $d(f) = d(1) \geq 0$ for $f \geq 1$. Then, we have the following stability estimate for the semi-discretization (19).

Lemma 4.3. *Let* $0 \leq f_i(0) \leq 1$ *for all* $i \in M$*. Then every solution* $(f_i(t))$ *of* (19) *fulfills*

$$0 \leq f_i(t) \leq 1, \quad \text{for all } i \in M \text{ and } t \geq 0.$$

Proof. Multiplication of (19) with $(f_i - 1)^+$ and summation by parts yields

$$\begin{aligned}
\frac{1}{2}\partial_t \sum_i |(f_i - 1)^+|^2 &= \frac{1}{(\Delta y)^2} \sum_i [m_{i+1}(f_{i+1} - f_i) - m_i(f_i - f_{i-1})]\,(f_i - 1)^+ \\
&= -\frac{1}{(\Delta y)^2} \sum_i m_i(f_i - f_{i-1}) \left[(f_i - 1)^+ - (f_{i-1} - 1)^+\right] \\
&\leq 0,
\end{aligned}$$

which can be verified by a direct computation.

Now Gronwall's Lemma implies due to $\sum_i |f_i(0) - 1)^+|^2 = 0$ that

$$\sum_i |(f_i(t) - 1)^+|^2 \equiv 0 \quad \text{for } t \geq 0,$$

i.e. $f_i(t) \leq 1$ for all $i \in M$ and $t \geq 0$.

The uniform lower bound $0 \leq f_i(t)$ for all $i \in M$ and $t \geq 0$ can be proven in analogy. □

Introducing a simple explicit Euler time discretization we end up again with a parabolic CFL condition as for the kinetic equation.

5. **Numerical experiments: Comparison of stochastic particle system and kinetic/diffusion equations.**

5.1. **Initialization.** For the numerical experiments we choose the following initial condition:

$$f^0(y) = \begin{cases} -|\frac{y}{\bar{L}^2}| + 1/\bar{L} & \text{if } |y| \leq \bar{L} \\ 0.0 & \text{otherwise} \end{cases} \tag{20}$$

where $\bar{L}$ is the radius of the compact support of the initial value which we assign to be 1.0 in the results presented below, cf. Figure 1. The calculations are carried out on the interval $y \in [-L, L] = [-3, 3]$ with $M = 101$ being the number of nodes for the discretization. All tests are preformed for the time horizon $T = 0.54$. Periodic boundary conditions are used. We compare three different solution methods. The reference solution is given by a Monte-Carlo simulation of the stochastic particle system. Moreover, the solution of the kinetic equation (3), as well as the solution of the diffusion equation with Green-Kubo diffusion coefficent using the method described in subsection 4.2, are plotted .

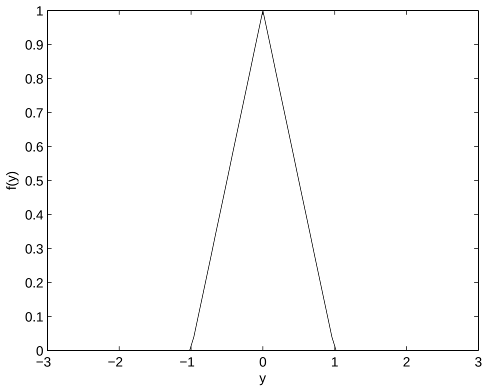

FIGURE 1. Initial conditions defined as a hat-function.

5.2. **Test scenarios.** For all test cases we plot the solution for the initial conditions in Figure 1. We investigate the solution of the kinetic equation (3), the macroscopic equation (5) with Green-Kubo coefficient and a Monte Carlo method for the stochastic particle system. As in section 2, we consider the following situations:

Example 1: $\alpha = -\beta$ with $\alpha > -2/3$.
As already mentioned, in this case we have a positive diffusion coefficient $d(f)$ which is not equal to the Green-Kubo one. The hopping rates are given by $\alpha_1' = \alpha_2' = 1$, $\alpha_3' = 1 + \alpha$, $\alpha_4' = 1 - \alpha$. In particular, we choose $\alpha = -1/2$. Then with the time rescale $t_{ref} = 3/2$ we get the original probabilites $\alpha_1 = 2/3 = \alpha_2, \alpha_3 = 1/3, \alpha_4 = 1$. Figure 2 shows a similar, but not equal, behaviour of the diffusion coefficients.
In Figure 3 we observe the evolution of the solution at fixed time $t = T$ for the stochastic particle system (MC), the kinetic equation (kinetic) and the diffusion equation with the Green Kubo diffusion coefficient (upwind).

Example 2: $\alpha = \beta$.
For this choice of parameters, the diffusion coefficient $d(f)$ becomes linear, namely: $d(f) = 2\alpha f + 1$. In this case $d(f)$ is equal to the Green-Kubo coefficient $d_{GK}(f)$. For our numerical comparison, we choose $\alpha = 1/2$. Then with the time rescale $t_{ref} = 2$ we have the probabilites $\alpha_1 = 1, \alpha_2 = 1/2, \alpha_3 = 3/4 = \alpha_4$. Figure 4 shows the same methods as above and verifies clearly the analytical results derived in section 2.

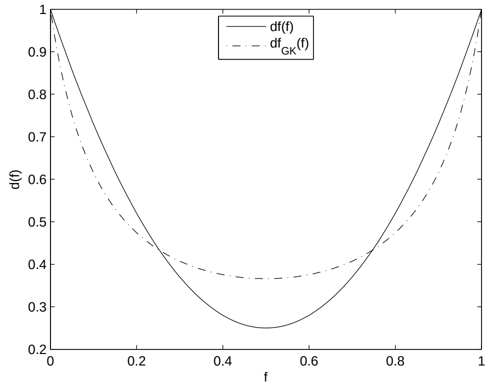

FIGURE 2. $d(f)$ and $d_{GK}(f)$ for case 1

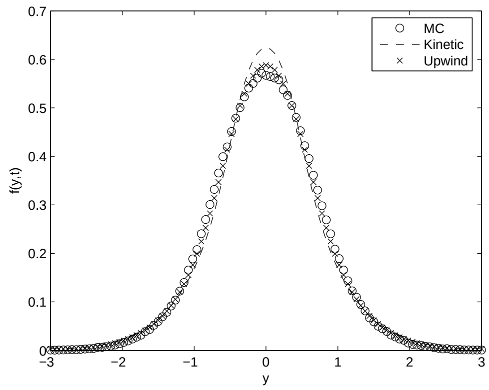

FIGURE 3. Nonnegative $d(f)$, weakly attractive potential

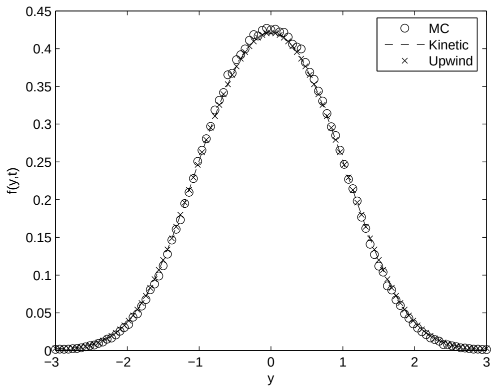

FIGURE 4. Example 2 with $d(f) = d_{GK}$

Example 3: $\alpha = -\beta$ with $\alpha < -2/3$.
This setting implies that the diffusion coefficient $d(f)$ becomes negative. We choose particularly $\alpha = -99/101$ and recover the probabilites $\alpha_1 = 101/200 = \alpha_2, \alpha_3 =$

$1/100, \alpha_4 = 1$ by the time rescale $t_{ref} = 200/101$. Figure 5 shows the diffusion coefficients where $d(f)$ is negative for $f \in (0.2, 0.8)$ and the Green-Kubo coefficient asymptotically approaches 0 away from the boundaries. The results are shown in Figure 6.

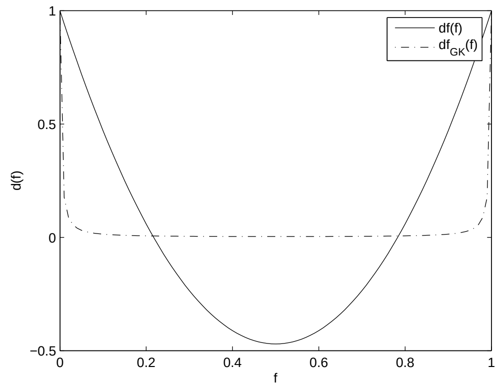

FIGURE 5. $d(f)$ and $d_{GK}(f)$ for case 3

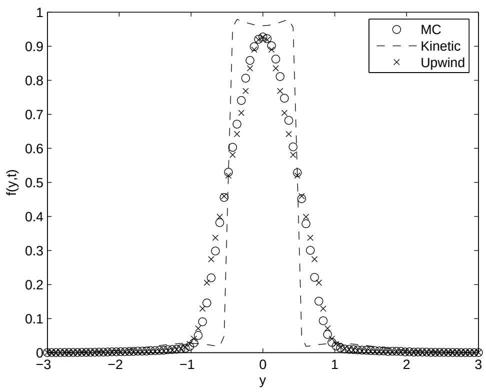

FIGURE 6. Time evolution for negative $d(f)$, strongly attractive potential

To conclude, we remark, that, as expected, only in Example 2, we obtain the same behaviour for the kinetic equation and the stochastic particle system. In all other situations the derivation of the kinetic equation from the stochastic particle system is not valid.

6. **Outlook.** The above results, in particular, the case $\alpha = \beta$ can be extended to two dimensions.

Theoretical results on the multi-dimensional problem in the case $\alpha = \beta$ are described in [6]. There, different parameters α_1 and α_2 are used for the respective directions. We consider the same situation.

The resulting kinetic equation is

$$\partial_t f_i = G(f) - L(f)$$

with

$$G(f) = G_1(f) + G_2(f), \quad L(f) = L_1(f) + L_2(f)$$

where, for $i = 1, 2$

$$G_i(f) = \overline{f}_i \Big(f_{i-1} + f_{i+1} + \alpha_i [f_{i+1} f_{i+2} + f_{i-1} f_{i-2} + 2 f_{i-1} f_{i+1}] \Big)$$

and

$$L_i(f) = f_i \Big(f_{i-1} + f_{i+1} + \alpha_i [f_{i-1} \overline{f}_{i+1} + \overline{f}_{i-1} f_{i+1} + \overline{f}_{i-1} f_{i-2} + \overline{f}_{i+1} f_{i+2}] \Big).$$

As in the one-dimensional case one can derive this equation from the particle system using the same procedure as in section 3. The resulting diffusion equation is, compare [6],

$$\partial_t f = \nabla \cdot (D(f) \cdot \nabla f)$$

with $D(f)$ being a diagonal matrix with entries

$$d_i(f) = 2\alpha_i f + 1, \; i = 1, 2.$$

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REFERENCES

[1] J. Adams, Z. Wang, and Y. Li, *Modeling Cu thin film growth*, Thin Solid Films, 365 (2000), pp. 201–210.
[2] T. Ala-Nissila, R. Ferrando, and S. Ying, *Collective and single particle diffusion on surfaces*, Adv. Phys., 51 (2002), pp. 949–1078.
[3] P. Degond, and A. Klar, *A relaxation approximation for transport equations in the diffusive limit.* Appl. Math. Lett., 15 (2002), pp. 131–135.
[4] B. Elton, C. Levermore, and G. Rodrigue, *Convergence of convective diffusive lattice Boltzmann methods*, SIAM J. Numer. Anal., 32 (1995), pp. 1327–1354.
[5] K.A. Fichthorn, and W.H. Weinberg, *Theoretical foundations of dynamical Monte-Carlo simulations*, J. Chem. Phys., 95 (1991), pp. 1090–1096.
[6] T. Funaki, K.Handa, and K. Uchiyama, *Hydrodynamic limit of one-dimensional exclusion processes with speed change*, Ann. Prob., 19 (1991), pp. 245–265.
[7] G. Gilmer, H. Huang, T. Rubia, J. Torre, and F. Baumann, *Lattice Monte Carlo models of thin film deposition*, Thin Solid Films, 365 (2000), pp. 189–200.
[8] M.Z. Guo, G.C. Papanicolaou, and S.R.S. Varadhan, *Nonlinear Diffusion limit for a system with nearest neighbour interactions*, Comm. Math. Phys., 118 (1988), pp. 31–59.
[9] A. Klar, and A. Unterreiter *Uniform stability of a finite difference scheme for transport equations in diffusive regimes*, SIAM J. Num. Anal., 40 (2002), pp. 891–913.
[10] M. Kotrla, *Numerical simulations in the theory of crystal growth*, Comp. Phys. Com., 97 (1996), pp. 82–100.
[11] MAPLE Version 8.0. Information available at URL http://www.scientific.de/maple.html.
[12] P. Rosenau, *Dynamics of dense lattices*, Phys. Rev. B, 36 (1987), pp. 5867–5876.
[13] H. Spohn, *Large scale dynamics of interacting particles*, Springer, New York, 1991.
[14] T. Witelski, *The structure of Internal Layers for Unstable Nonlinear Diffusion Equations*, Studies in Appl. Math., 97 (1996), pp. 277–300.
[15] T. Witelski, D. Schaeffer, and M. Shearer, *A discrete model for an ill-posed nonlinear parabolic PDE*, Physica D, 160 (2001), pp. 189–221.
[16] W. Zwerger, *The density dependence of the diffusion constant in interacting lattice gases*, Z. Phys.B, 42 (1981), pp. 333–347.

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