Excluded-volume effects in the diffusion of hard spheres

Maria Bruna-Estrach and S. Jonathan Chapman
University of Oxford, Mathematical Institute, 24-29 St. Giles', Oxford, OX1 3LB, United Kingdom
(Dated: December 14, 2010)

Excluded-volume effects can play an important role in determining transport properties in diffusion of particles through crowded environments. Here, the diffusion of finite-sized hard-core interacting particles is considered systematically using the method of matched asymptotic expansions. The result is a nonlinear diffusion equation for the one-particle distribution function, with crowding effects enhancing the overall diffusion rate. Stochastic simulations of the full particle system are shown to compare well with the solution of this equation for two examples.

PACS numbers: 05.10.Gg, 02.30.Jr, 02.30.Mv, 05.40.Fb

Recently there has been an increasing interest in understanding particle transport in crowded environments [1]. Crowding is important in many biological processes, including diffusion through ion channels [2], inside the cell cytoplasm (macromolecular crowding) [3–5] and in chemotaxis [6], and can have a significant impact on the thermodynamics and kinetics of biological processes such as macromolecular reaction rates and the folding of proteins [3–5, 7]. Finite-size effects are also important when considering the combustion of powders [8], collective behaviour (*e.g.* animal flocks) [9] and granular gases [10].

Excluded-volume or steric interactions arise from the mutual impenetrability of finite-size particles (see Fig. 1). For one-dimensional configurations, such as channels, the single-file diffusion of hard-core particles can be solved exactly by mapping it to the classical diffusion of point-particles [11, 12]. However, the situation in higher dimensions is more challenging.

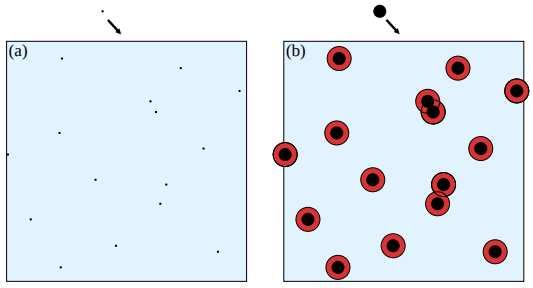

FIG. 1. (color online). Excluded (red and black) and available (blue) area in a solution of black particles for the placement of an additional test particle. (a) The area available with point particles is the whole domain. (b) The area available (to the *center* of the test particle) with finite-size particles is reduced. Modified from Minton [7].

Batchelor [13] models Brownian diffusion of particles with hydrodynamic interaction using generalized Einstein relations to find a concentration dependent correction to the diffusion coefficient. Felderhof [14] considers the same problem through an analysis of the Fokker-Planck equation, and includes both excluded volume and hydrodynamic effects. His analysis is based on the thermodynamic limit (in which the number of particles N and the system volume V tend to infinity, with the concentration N/V fixed), and is valid only for a small perturbation from the equilibrium concentration.

Muramatsu and Minton [15] use a simple model to calculate the diffusion coefficient of hard spheres by estimating the probability that the target volume for a step in a random walk is free of any macromolecules. Other authors model excluded volume phenomenologically by introducing a particle pressure, and an equation of state in which the compressibility is reduced as the concentration increases [16].

Another popular approach is to consider lattice models, in which a particle can only move to a site if it is presently unoccupied. Such an approach is used to model diffusion of multiple species with size exclusion effects in [17] or to model the effect of crowding on diffusion-limited reaction in [18].

The preceding approaches are all either phenomenological in nature, restricted to small perturbations from a uniform concentration, or based on the thermodynamic limit in which the number of particles tends to infinity. Here we consider a finite number of finite-sized particles diffusing in a box of fixed size. We perform an asymptotic analysis of the associated Fokker-Planck equation in the limit that the volume fraction of particles is small. Our analysis is systematic, using the method of matched asymptotic expansions, but is not appropriate for concentrations close to the jamming limit.

In order to focus on steric effects, we suppose that there are no electrostatic or hydrodynamic interaction forces between particles. We work in d dimensions, where d is either 2 or 3. Thus our starting point is a system of N identical hard core diffusing and interacting spheres (or disks), each with constant diffusion coefficient D and diameter K, in a bounded domain Ω in $\mathbb{R}^d$ of typical diameter L. By nondimensionalizing length with L and time with L^2/D, the size of the domain and the diffusion coefficient may be normalized to unity, while the diameter of the particles becomes $\epsilon = K/L$. We assume that the particles occupy a small volume fraction, so that $N\epsilon^d \ll 1$. We denote the centres of the particles by $\mathbf{X}_i(t) \in \Omega$ at time $t \geq 0$, where $1 \leq i \leq N$ [19]. Each centre evolves

according to the stochastic differential equation (SDE)

$$\mathrm{d}\mathbf{X}_i \equiv \sqrt{2}\,\mathrm{d}\mathbf{B}_i + \mathbf{f}_i\,\mathrm{d}t, \qquad 1 \le i \le N, \tag{1}$$

where the $\mathbf{B}_i$ are N independent d-dimensional standard Brownian motions and $\mathbf{f}_i$ is the external force on the ith particle. In general this force may include both inter-particle and external interactions, such as electromagnetic, friction, convection and potential forces, in which case $\mathbf{f}_i$ depends on the positions of all the particles $\vec{X} = (\mathbf{X}_1, \ldots, \mathbf{X}_N)$. While soft-core steric effects can also be built into $\mathbf{f}_i$, hard-core collisions can be more easily expressed as reflective boundary conditions on the "collision surfaces" $r = ||\mathbf{X}_i - \mathbf{X}_j|| = \epsilon$, with $1 \le i < j \le N$. Since we are focussing on hard-core particle interactions, we restrict ourselves to other external forces of the form

$$\vec{F}(\vec{X}) = [\mathbf{f}(\mathbf{X}_1), \ldots, \mathbf{f}(\mathbf{X}_N)], \tag{2}$$

where $\mathbf{f} : \Omega \to \mathbb{R}^d$ acts identically on all N particles. We suppose that the initial positions $\mathbf{X}_i(0)$ are independently identically distributed.

Let $P(\vec{x}, t)$ be the joint probability density function of the N particles. Then, by the Itô formula, $P(\vec{x}, t)$ evolves according to the linear Fokker-Planck partial differential equation (PDE)

$$\frac{\partial P}{\partial t} = \nabla_{\vec{x}} \cdot \left[\nabla_{\vec{x}}\, P - \vec{F}(\vec{x})\, P\right] \quad \text{in} \quad \Omega_\epsilon^N, \tag{3a}$$

where $\nabla_{\vec{x}}$ and $\nabla_{\vec{x}}\cdot$ respectively stand for the gradient and divergence operators with respect to the N-particle position vector $\vec{x} = (\mathbf{x}_1, \ldots, \mathbf{x}_N) \in \Omega^N$. Note that because of steric effects, (3) is not defined in Ω^N but in its "hollow form" $\Omega_\epsilon^N = \Omega^N \setminus \mathcal{B}_\epsilon$, where $\mathcal{B}_\epsilon = \{\vec{x} \in \Omega^N : \exists i \ne j \text{ such that } ||\mathbf{x}_i - \mathbf{x}_j|| \le \epsilon\}$ is the set of all illegal configurations (with at least one overlap). On the collision surfaces $\partial\Omega_\epsilon^N$ we have the reflecting boundary condition

$$\left[\nabla_{\vec{x}}\, P - \vec{F}(\vec{x})\, P\right] \cdot \vec{n} = 0 \quad \text{on} \quad \partial\Omega_\epsilon^N, \tag{3b}$$

where $\vec{n} \in \mathcal{S}^{dN-1}$ denotes the unit outward normal.

Although linear, the PDE model (3) is very high-dimensional, and it is impractical to solve it directly. Since all the particles are identical and P is invariant to a switch of particle labels, we are interested mainly in the marginal distribution function of the first particle, given by $p(\mathbf{x}_1, t) = \int P(\vec{x}, t)\ \mathrm{d}\mathbf{x}_2 \ldots \mathrm{d}\mathbf{x}_N$. We aim to reduce the high-dimensional PDE for P to a low-dimensional PDE for p through a systematic asymptotic expansion as $\epsilon \to 0$. In the particular case of point-particles ($\epsilon = 0$) the model reduction is straightforward. In this case the N particles are independent and the domain is $\Omega_\epsilon^N \equiv \Omega^N$ (no holes), which implies that the internal boundary conditions in (3b) vanish. Therefore $P(\vec{x}, t) = \prod_{i=1}^N p(\mathbf{x}_i, t)$, and

$$\frac{\partial p}{\partial t}(\mathbf{x}_1, t) = \nabla_{\mathbf{x}_1} \cdot [\nabla_{\mathbf{x}_1}\, p - \mathbf{f}(\mathbf{x}_1)\, p] \quad \text{in} \quad \Omega, \tag{4a}$$

$$0 = [\nabla_{\mathbf{x}_1}\, p - \mathbf{f}(\mathbf{x}_1)\, p] \cdot \hat{\mathbf{n}}_1 \quad \text{on} \quad \partial\Omega, \tag{4b}$$

where $\hat{\mathbf{n}}_1$ is the outward unit normal to $\partial\Omega$.

When $\epsilon > 0$, the internal boundary conditions in (3b) mean the particles are no longer independent. When we integrate (3) over $\mathbf{x}_2$, …, $\mathbf{x}_N$ and apply the divergence theorem we end up with surface integrals over the collision surfaces, on which P must be evaluated. However, when the particle volume fraction is small, the volume in Ω_ϵ^N occupied by configurations in which three or more particles are close is small $[O(\epsilon^{2d}N^2)]$ compared to those in which two particles alone are in proximity $[O(\epsilon^d N)]$. Thus the dominant contribution to these "collision integrals" corresponds to two-particle collisions. We illustrate our approach for $N = 2$; since two-particle collisions dominate the extension to arbitrary N is straightforward.

For two particles at positions $\mathbf{x}_1$ and $\mathbf{x}_2$, Eq. (3a) reads

$$\begin{aligned}\frac{\partial P}{\partial t}(\mathbf{x}_1, \mathbf{x}_2, t) = \ & \nabla_{\mathbf{x}_1} \cdot [\nabla_{\mathbf{x}_1} P - \mathbf{f}(\mathbf{x}_1) P] \\ & + \nabla_{\mathbf{x}_2} \cdot [\nabla_{\mathbf{x}_2} P - \mathbf{f}(\mathbf{x}_2) P]\,,\end{aligned} \tag{5a}$$

for $(\mathbf{x}_1, \mathbf{x}_2) \in \Omega_\epsilon^2$, and the boundary condition (3b) reads

$$[\nabla_{\mathbf{x}_1} P - \mathbf{f}(\mathbf{x}_1) P] \cdot \hat{\mathbf{n}}_1 + [\nabla_{\mathbf{x}_2} P - \mathbf{f}(\mathbf{x}_2) P] \cdot \hat{\mathbf{n}}_2 = 0, \tag{5b}$$

on $\mathbf{x}_i \in \partial\Omega$ and $||\mathbf{x}_1 - \mathbf{x}_2|| = \epsilon$. Here $\hat{\mathbf{n}}_i = \mathbf{n}_i/|\mathbf{n}_i|$, where $\mathbf{n}_i$ is the component of the normal vector $\vec{n}$ corresponding to the $i-$th particle, $\vec{n} = (\mathbf{n}_1, \mathbf{n}_2)$. We note that $\hat{\mathbf{n}}_1 = 0$ on $\mathbf{x}_2 \in \partial\Omega$, and that $\hat{\mathbf{n}}_1 = -\hat{\mathbf{n}}_2$ on $||\mathbf{x}_1 - \mathbf{x}_2|| = \epsilon$.

We denote by $\Omega(\mathbf{x}_1)$ the region available to particle 2 when particle 1 is at $\mathbf{x}_1$, namely $\Omega(\mathbf{x}_1) = \Omega \backslash B_\epsilon(\mathbf{x}_1)$. Note that when the distance between $\mathbf{x}_1$ and $\partial\Omega$ is less than ϵ the area $|\Omega(\mathbf{x}_1)|$ increases. This creates a boundary layer of width ϵ around $\partial\Omega$ where there exists a wall-particle-particle interaction (three-body interaction). Since the dimensions of the container are much larger than the particle diameter these interactions are higher-order and we may safely ignore them and take $|\Omega(\mathbf{x}_1)|$ constant [20]. Integrating Eq. (5a) over $\Omega(\mathbf{x}_1)$ yields

$$\begin{aligned}\frac{\partial p}{\partial t}(\mathbf{x}_1, t) = \ & \nabla_{\mathbf{x}_1} \cdot [\nabla_{\mathbf{x}_1}\, p - \mathbf{f}(\mathbf{x}_1)\, p] \\ & + \int_{\partial B_\epsilon(\mathbf{x}_1)} [\mathbf{f}(\mathbf{x}_1)\, P - 2\nabla_{\mathbf{x}_1} P - \nabla_{\mathbf{x}_2} P] \cdot \hat{\mathbf{n}}_2\, \mathrm{d}S_2 \\ & + \int_{\partial\Omega \cup \partial B_\epsilon(\mathbf{x}_1)} [\nabla_{\mathbf{x}_2}\, P - \mathbf{f}(\mathbf{x}_2)\, P] \cdot \hat{\mathbf{n}}_2\, \mathrm{d}S_2\end{aligned} \tag{6}$$

The first integral in (6) comes from switching the order of integration with respect to $\mathbf{x}_2$ and differentiation with respect to $\mathbf{x}_1$ using the transport theorem; the second comes from using the divergence theorem on the derivatives in $\mathbf{x}_2$. Using (5b) and rearranging we find

$$\begin{aligned}\frac{\partial p}{\partial t}(\mathbf{x}_1, t) = \ & \nabla_{\mathbf{x}_1} \cdot [\nabla_{\mathbf{x}_1}\, p - \mathbf{f}(\mathbf{x}_1)\, p] \\ & + \int_{\partial B_\epsilon(\mathbf{x}_1)} \{-2\nabla_{\mathbf{x}_1} P + P\,[\mathbf{f}(\mathbf{x}_1) - \mathbf{f}(\mathbf{x}_2)]\} \cdot \hat{\mathbf{n}}_2\, \mathrm{d}S_2.\end{aligned} \tag{7}$$

Because the pairwise particle interaction is localized near the collision surface $\partial B_\epsilon(\mathbf{x}_1)$ we can determine it

using the method of matched asymptotic expansions [21]. We suppose that when two particles are far apart ($||\mathbf{x}_1 - \mathbf{x}_2|| \gg \epsilon$) they are independent, whereas when they are close to each other ($||\mathbf{x}_1 - \mathbf{x}_2|| \sim \epsilon$) they are correlated. We designate these two regions of configuration space the outer region and inner region, respectively.

In the inner region, we set $\mathbf{x}_1 = \tilde{\mathbf{x}}_1$ and $\mathbf{x}_2 = \tilde{\mathbf{x}}_1 + \epsilon\tilde{\mathbf{x}}$ and define $\tilde{P}(\tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}, t) = P(\mathbf{x}_1, \mathbf{x}_2, t)$ to give

$$\epsilon^2 \frac{\partial \tilde{P}}{\partial t}(\tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}, t) = 2\nabla^2_{\tilde{\mathbf{x}}} \tilde{P} - \epsilon^2 \nabla_{\tilde{\mathbf{x}}_1} \cdot \left[\mathbf{f}(\tilde{\mathbf{x}}_1)\tilde{P}\right] + \epsilon^2 \nabla^2_{\tilde{\mathbf{x}}_1} \tilde{P} + \epsilon \nabla_{\tilde{\mathbf{x}}} \cdot \left\{ \left[\mathbf{f}(\tilde{\mathbf{x}}_1) - \mathbf{f}(\tilde{\mathbf{x}}_1 + \epsilon\tilde{\mathbf{x}})\right] \tilde{P} \right\} - 2\epsilon \nabla_{\tilde{\mathbf{x}}_1} \cdot \nabla_{\tilde{\mathbf{x}}} \tilde{P}, \quad (8a)$$

with

$$2\tilde{\mathbf{x}} \cdot \nabla_{\tilde{\mathbf{x}}} \tilde{P} = \epsilon\, \tilde{\mathbf{x}} \cdot \left\{ \nabla_{\tilde{\mathbf{x}}_1} \tilde{P} + \left[\mathbf{f}(\tilde{\mathbf{x}}_1 + \epsilon\tilde{\mathbf{x}}) - \mathbf{f}(\tilde{\mathbf{x}}_1)\right] \tilde{P} \right\}, \quad (8b)$$

on $||\tilde{\mathbf{x}}|| = 1$. Here we assume that $\tilde{\mathbf{x}}_1$ is not close to $\partial\Omega$; the region in which the particles are close to each other and the boundary is even smaller, and will affect only the higher-order terms. In addition to (8b) the inner solution must match with the outer solution as $\tilde{\mathbf{x}} \to \infty$. In the outer region, by independence,

$$P(\mathbf{x}_1, \mathbf{x}_2, t) = q(\mathbf{x}_1, t) q(\mathbf{x}_2, t),$$

for some function $q(\mathbf{x}, t)$. The normalization condition on P gives $q(\mathbf{x}_1, t) = p(\mathbf{x}_1, t) + \mathcal{O}(\epsilon^d)$. Expanding this outer solution in inner variables gives

$$P(\mathbf{x}_1, \mathbf{x}_2, t) = q(\tilde{\mathbf{x}}_1, t) q(\tilde{\mathbf{x}}_1 + \epsilon\tilde{\mathbf{x}}) \sim q^2(\tilde{\mathbf{x}}_1, t) + \epsilon q(\tilde{\mathbf{x}}_1)\, \tilde{\mathbf{x}} \cdot \nabla_{\tilde{\mathbf{x}}_1} q(\tilde{\mathbf{x}}_1) + \cdots. \quad (8c)$$

Expanding $\tilde{P}$ in powers of ϵ, and solving (8b), (8b) with the matching condition (8c) we find that the solution in the inner region is simply

$$\tilde{P}(\tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}, t) \sim q^2(\tilde{\mathbf{x}}_1, t) + \epsilon q(\tilde{\mathbf{x}}_1)\, \tilde{\mathbf{x}} \cdot \nabla_{\tilde{\mathbf{x}}_1} q(\tilde{\mathbf{x}}_1) + \cdots. \quad (9)$$

Using this solution to evaluate the integrals in (7) we find, to $O(\epsilon^d)$,

$$\frac{\partial p}{\partial t}(\mathbf{x}_1, t) = \nabla_{\mathbf{x}_1} \cdot \left[\nabla_{\mathbf{x}_1} \left(p + \alpha_d \epsilon^d p^2 \right) - \mathbf{f}(\mathbf{x}_1)\, p \right], \quad (10)$$

where $\alpha_2 = \pi/2$ and $\alpha_3 = 2\pi/3$. The extension from two particles to N particles is straightforward up to $O(\epsilon^d)$, since at this order only pairwise interactions need to be considered. Particle 1 has $(N-1)$ inner regions, one with each of the remaining particles. A similar procedure shows that the marginal distribution function satisfies

$$\frac{\partial p}{\partial t}(\mathbf{x}_1, t) = \nabla_{\mathbf{x}_1} \cdot \left\{ \nabla_{\mathbf{x}_1} \left[p + \alpha_d (N-1) \epsilon^d p^2 \right] - \mathbf{f}(\mathbf{x}_1)\, p \right\}, \quad (11a)$$

$$0 = \left[\nabla_{\mathbf{x}_1} p - \mathbf{f}(\mathbf{x}_1)\, p\right] \cdot \mathbf{n}_1 \quad \text{on} \quad \partial\Omega. \quad (11b)$$

We see that steric interactions lead to a concentration-dependent diffusion coefficient, with the additional term proportional to the excluded volume. Equation (11a) is consistent with that derived by Felderhof [14], but extends it to situations in which p is not close to uniform.

In (11) we have only included the leading-order nonlinear term due to steric effects. There will be correction terms of $O(\epsilon^{d+1}N)$ due to higher-order terms in the two-particle inner solution (9), as well as new inner regions where three particles $[O(\epsilon^{2d}N^2)]$, or two particles and the boundary $[O(\epsilon^{d+1}N)]$, are close. Because our asymptotic expansion is systematic, these correction terms could in principle be calculated.

In order to assess the validity of (11) we compare its solution $p(\mathbf{x}_1, t)$ (obtained by a simple finite difference method) with Monte Carlo (MC) simulations of the $2N$-coupled SDE (1) in two dimensions. The particle-particle (and particle-wall) overlaps are treated as in [22]. To test the importance of steric interactions, we also compare with the corresponding solutions with $\epsilon = 0$.

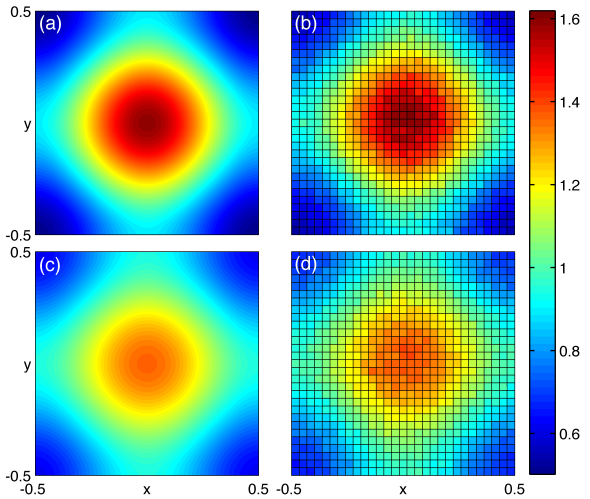

FIG. 2. (color online). Marginal distribution function $p(\mathbf{x}_1, t)$ at time $t = 0.05$ with normally distributed initial data and $N = 400$. (a) Solution $p(\mathbf{x}_1, t)$ of (4) for point particles ($\epsilon = 0$). (b) Histogram for $\epsilon = 0$. (c) Solution $p(\mathbf{x}_1, t)$ of (11) for finite-sized particles ($\epsilon = 0.01$). (d) Histogram for $\epsilon = 0.01$. Histograms computed from 10^4 realizations of (1) with $\Delta t = 10^{-5}$. All four plots have the same color bar.

In Fig. 2 we show the results of a time-dependent simulation with $\mathbf{f} \equiv 0$, $\Omega = [-\frac{1}{2}, \frac{1}{2}]^2$, $\epsilon = 0.01$, $N = 400$, for which the initial distribution is a Gaussian of zero mean and variance 0.05 (normalized so that its integral over Ω is one); the figures correspond to time $t = 0.05$. The simulation time-step Δt is chosen such that almost no collisions are missed. The theoretical predictions for both point and finite-size particles compare very well with their simulation counterparts, while steric effects are clearly appreciable even though the volume fraction of particles is only 0.0314. The initial profile spreads faster when steric effects are included [Fig. 2(c)] than when they are not [Fig. 2(a)], indicating that the overall diffusion is enhanced.

When the force field $\mathbf{f}$ is the gradient of a potential, $\mathbf{f}(\mathbf{x}_1) = -\nabla_{\mathbf{x}_1} V(\mathbf{x}_1)$, we may write $\frac{\partial p}{\partial t} + \nabla_{\mathbf{x}_1} \cdot (p\mathbf{u}) = 0$, with $\mathbf{u} = -\nabla_{\mathbf{x}_1} \left[\log p + 2\alpha_d (N-1)\epsilon^d p + V(\mathbf{x}_1)\right]$. Then the stationary distribution, which we denote $p_s(\mathbf{x}_1)$, is obtained by solving [23]

$$\log p_s(\mathbf{x}_1) + 2\alpha_d (N-1)\epsilon^d p_s(\mathbf{x}_1) + V(\mathbf{x}_1) = C, \quad (12)$$

with the constant C determined by the normalisation condition on p_s. For our second example we consider the volcano-shaped potential $V(\mathbf{x}_1) = -4.77\, \mathrm{e}^{-100||\mathbf{x}_1||^2} + 3.58\, \mathrm{e}^{-50||\mathbf{x}_1||^2}$ and we compare the stationary distribution p_s predicted by (12) with simulations using the Metropolis-Hastings (M-H) algorithm [24]. Figure 3 shows the model and simulation results with $N = 1000$ and Ω and ϵ as in Fig. 2 for both point and finite-size particles. In this case there is competition between the potential well and steric repulsion: the particle density inside the well is reduced for finite-size particles. Again, the agreement between the model (12) and the stochastic simulations is excellent.

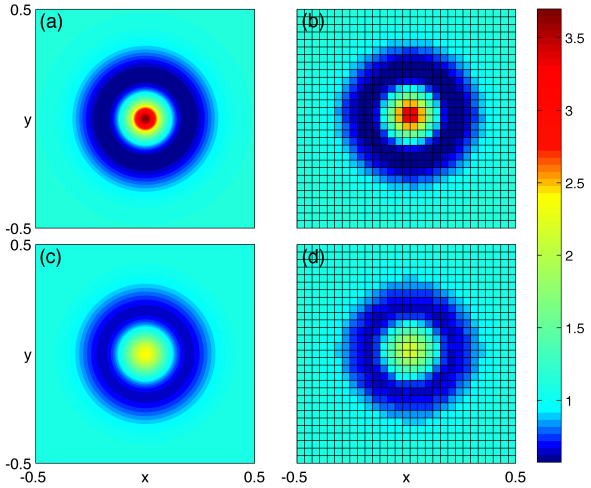

FIG. 3. (color online). Stationary marginal distribution function $p_s(\mathbf{x}_1)$ under the external potential V for point particles and finite-size particles, with $N = 1000$. (a) Point particles, $p_s \propto e^{-V}$. (b) Histogram for $\epsilon = 0$. (c) Finite-size particles p_s from (12) ($\epsilon = 0.01$). (d) Histogram for $\epsilon = 0.01$. Histograms computed with 10^9 steps of the M-H algorithm. All four plots have the same color bar.

We have derived systematically a nonlinear diffusion equation which describes steric interactions in the limit of small but finite particle volume fraction. Our method justifies for example the ansatz made in [25] to account for the finite size of the cells and prevent aggregation, and unlike [14, 26] does not rely on a closure assumption.

The method was implemented here in its simplest setting (hard-core identical spherical particles with an external potential) but it can be extended in many directions. Particles of different size or shape could easily be incorporated, while the hard-core interaction between particles can be replaced by any short-range soft-core interaction.

On the other hand, incorporating long range effects such as chemotaxis or electrostatic interactions is more challenging; in such cases a system size expansion is likely to be needed in addition to a small particle expansion.

MB expresses her cordial thanks to the Isaac Newton Institute for Mathematical Sciences for its hospitality during the preparation of the present paper. MB holds an EPSRC studentship.

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[19] Note that Ω is the space available to a particle centre, which is slightly smaller than the container due to the finite size of the particles.
[20] This would not be the case in a channel-like domain, for instance. If $\Omega = [0,1] \times [0,L]$ with $L = O(\epsilon)$, the wall-particle-particle interactions would become important.
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