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One-dimensional drift-diffusion between two absorbing boundaries: application to granular segregation

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Abstract

Motivated by a novel method for granular segregation, we analyse the one-dimensional drift-diffusion between two absorbing boundaries. The time evolution of the probability distribution and the rate of absorption are given by explicit formulae; the splitting probability and the mean first-passage time are also calculated. Applying the results we find optimal parameters for segregating binary granular mixtures.

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1. Introduction

The diffusion phenomena have been one of the most intensively studied fields in statistical physics. A number of textbooks have been written in this field, and in many of them the one-dimensional case is discussed in detail [1–4]. The drift-diffusion equation has been studied in many different contexts even recently [5–8]. Still, according to our knowledge, the problem of one-dimensional drift-diffusion between two absorbing boundaries has not been completely solved.

The need for the solution of this problem arose when we investigated the motion of a granular particle in a vertically vibrated ratchet by means of a 2D computer simulation (see figure 1).

In the simulation we used an event-driven algorithm with a hard-sphere collision model [12, 13]. The particles can rotate around the axis going through their centre and perpendicular to the plane of the box; their moment of inertia is $2/5\,mr^2$ about their centre. Since the mass of the particles does not play a role in collisions with the base but only in binary collisions, it is enough to specify that the particles have the same mass density, so $m \propto r^3$. (For a detailed description of the setup, see [14].) We found that the horizontal motion of one particle can be well approximated as drift-diffusion (see figures 2 and 3), and

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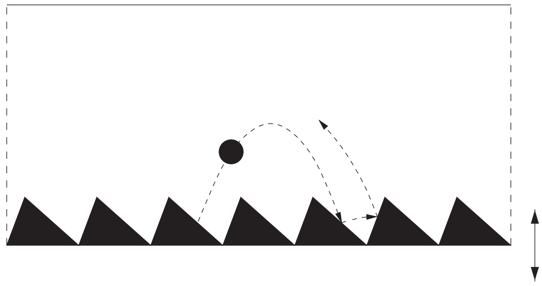

Figure 1. The setup of the one-particle simulation. The two-dimensional box has an asymmetrical sawtooth-shaped base, which is sinusoidally vibrated in the vertical direction with amplitude A and frequency f. The shape of the sawtooth can be described by three parameters: width w, height h and asymmetry parameter a, which is the ratio of the projection of the left-hand edge onto the base and w. The particle has five parameters: mass m, radius r, coefficient of restitution ε, friction coefficient μ and maximum tangential restitution coefficient β_0. The boundary condition can be either periodic, reflective or absorbing.

the parameters of the diffusion process, i.e. the average velocity and the diffusion constant, depend on the parameters of the particle and the ratchet[4]. According to our results, it is possible that the average velocities of two kinds of particles in the same system have opposite directions. If the boundaries are open (i.e. the absorbing boundary condition is applied), then this setup is capable of segregating a binary granular mixture of these particles provided that the load rate is chosen so that only a few particles are in the system at one time (in this case the interaction between the particles can be neglected, and we do not have the problem that the transport velocity also depends on the number of particles). Note that in this setup the segregation is due to the interaction between the ratchet and the individual particles, while in other granular segregation phenomena the segregation is primarily due to the interaction between the particles, involving many-body collective effects [9–11]. We need the theoretical description to predict, for example, the quality of the segregation or the highest possible load rate, and to further improve the quality by choosing optimal parameters, such as where to load the granular mixture along the box. The results of the granular binary mixture segregation will be published elsewhere.

2. The diffusion equation with bias

The dynamics of the diffusing particle is characterized by the diffusion constant D and mean velocity $v \neq 0$, which is the result of an external field. (The results for the $v = 0$ case will be presented later.) The diffusion equation then reads $\partial_t p(x,t) = D\partial_x^2 p(x,t) - v\partial_x p(x,t)$. The relevant quantities are D and v, which define a characteristic time $t^* = D/v^2$ and a characteristic length $l^* = D/v$. We use t^* and l^* to non-dimensionalize the problem; all quantities are dimensionless in the rest of this section. The dimensionless diffusion equation is

$$\partial_t p(x,t) = \partial_x^2 p(x,t) - \partial_x p(x,t) \tag{1}$$

with initial condition $p(x,0) = p_0(x)$ for $0 \leqslant x \leqslant L$, and boundary condition $p(0,t) = p(L,t) = 0$ for $t \geqslant 0$, where L is the system width, and we start at $t = 0$. The absorbing boundary condition is equivalent to the probability being zero at the boundaries [3]. Let us

[4] The detailed analysis of the one-particle motion and the segregation of binary granular mixtures using this method will be published elsewhere.

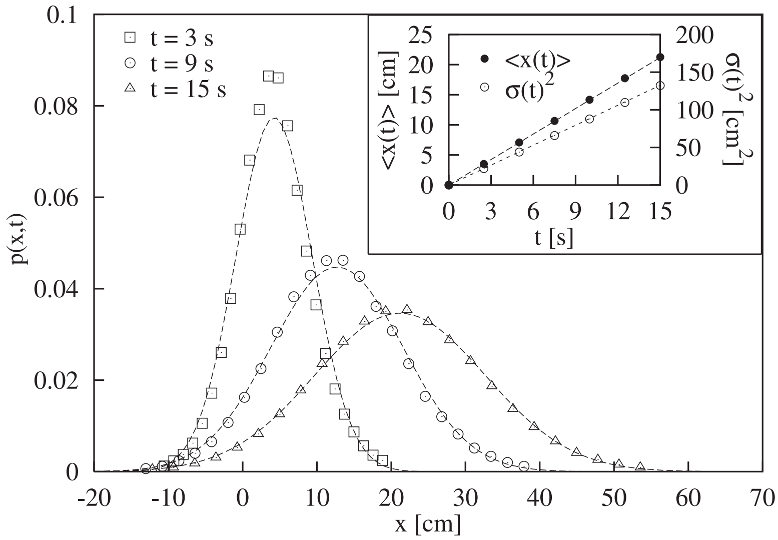

Figure 2. Simulation result: the probability distribution of the horizontal position of a particle which is started from $x = 0$ at zero time, in an infinitely wide system (natural boundary condition). The dashed curves show the theoretical prediction $\frac{1}{\sqrt{4\pi Dt}}\mathrm{e}^{-\frac{(x-vt)^2}{4Dt}}$, which is the probability distribution of a drift–diffusing particle in one dimension. The velocity v and diffusion constant D are determined by line fitting: $\langle x(t)\rangle = vt$ and $\sigma(t)^2 = 2Dt$ (see inset), where $\sigma(t)^2 = \langle x(t)^2\rangle - \langle x(t)\rangle^2$. The fitted values are $v = 1.42$ cm s^{-1} and $D = 4.42$ cm^2 s^{-1}. The parameters of the simulation are the following: $A = 2$ mm, $f = 28$ Hz, $w = 6$ mm, $h = 8.5$ mm, $a = 0.07$, $r = 1.2$ mm, $\varepsilon = 0.45$, $\mu = 0.1$ and $\beta_0 = 0$.

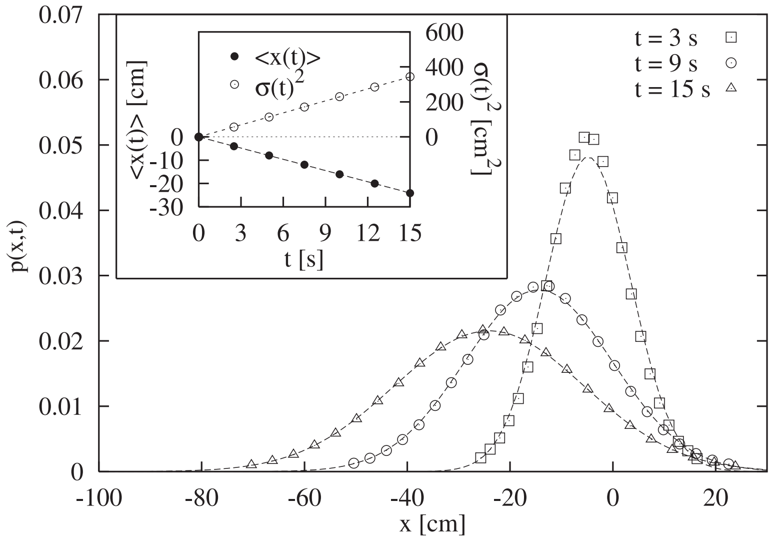

Figure 3. The same as in figure 2, except that the restitution coefficient of the particle is $\varepsilon = 0.6$. The fitted diffusion parameters are $v = -1.60$ cm s^{-1} and $D = 11.43$ cm^2 s^{-1}. Note that the direction of the velocity is the opposite, which makes possible the segregation of a granular mixture consisting of particles with $\varepsilon = 0.45$ and 0.6.

define operator $F = \partial_x^2 - \partial_x$ with $\mathcal{D}_F = \{\phi(x)|\phi(0) = \phi(L) = 0\} \cap \mathcal{D}^2$, where $\mathcal{D}^2$ is the set of twice-differentiable functions. If $\phi_\lambda \in \mathcal{D}_F$ is an eigenfunction of F with eigenvalue λ, then $\exp(\lambda t)\phi_\lambda$ is a solution of (1). If we had an orthonormal and complete eigensystem of F, we could give the solution of (1) immediately. It is a problem that F is not Hermitian, as far as the usual scalar product $\int_0^L \phi_1^*(x)\phi_2(x)\,\mathrm{d}x$ is concerned. However, F is Hermitian if the scalar product is calculated with kernel function e^{-x}: $\langle\phi_1|\phi_2\rangle \equiv \int_0^L \mathrm{e}^{-x}\phi_1^*(x)\phi_2(x)\,\mathrm{d}x$. It is useful to write F in the form $F = \mathrm{e}^x\partial_x\mathrm{e}^{-x}\partial_x$. The verification of the fact that F is Hermitian with scalar product $\langle\cdot|\cdot\rangle$, i.e. $\langle\phi_1|F\phi_2\rangle = \langle F\phi_1|\phi_2\rangle$, is straightforward: the effect of operator F can be shifted from ϕ_2 to ϕ_1 using two consecutive partial integrations, during which the surface terms disappear, because $\phi_1(x)$ and $\phi_2(x)$ are zero on the borders. Since F is Hermitian with scalar product $\langle\cdot|\cdot\rangle$, it has a complete orthonormal eigenfunction system with real eigenvalues. It is straightforward to verify that the eigenfuctions are $p_k(x) = \sqrt{\frac{2}{L}}\mathrm{e}^{x/2}\sin\left(\frac{k\pi}{L}x\right)$ with eigenvalues $\lambda_k = -\left(\frac{k\pi}{L}\right)^2 - \frac{1}{4}$ ($k \in \mathbb{N}^+$). The solution of (1), if $p^0(x)$ is the initial probability distribution, is $p(x,t) = \sum_{k=1}^\infty \langle p^0|p_k\rangle p_k(x)\mathrm{e}^{\lambda_k t}$. In the rest of the paper we investigate the case when the initial distribution is a Dirac delta-function at αL ($0 < \alpha < 1$). The weights are then $\langle\delta(x-\alpha L)|p_k\rangle = \sqrt{\frac{2}{L}}\mathrm{e}^{-\frac{\alpha L}{2}}\sin(k\pi\alpha)$, and the probability distribution is given by

$$\begin{aligned} p(x,t) &= \frac{2}{L}\mathrm{e}^{\frac{x-\alpha L}{2}}\sum_{k=1}^{\infty}\sin(k\pi\alpha)\sin\left(\frac{k\pi}{L}x\right)\mathrm{e}^{-\left[\left(\frac{k\pi}{L}\right)^2+\frac{1}{4}\right]t} \\ &= \frac{1}{2L}\mathrm{e}^{\frac{x-\alpha L}{2}-\frac{t}{4}}\left\{\vartheta_3\left[\left(\alpha-\frac{x}{L}\right)\frac{\pi}{2}, z(t)\right] - \vartheta_3\left[\left(\alpha+\frac{x}{L}\right)\frac{\pi}{2}, z(t)\right]\right\} \end{aligned} \tag{2}$$

where we introduce the notation $z(t) = \mathrm{e}^{-\frac{\pi^2}{L^2}t}$ and the theta function $\vartheta_3(r,q) = 1 + 2\sum_{k=1}^\infty \cos(2rk)q^{k^2}$ to obtain a closed form [15]. An important quantity is the rate of absorption, i.e. the probability current at the borders. Using the notation $\vartheta_3'(r,q) \equiv \partial_{\tilde{r}}\vartheta_3(\tilde{r},q)|_{\tilde{r}=r}$, the probability current $j(x,t) = -\partial_x p(x,t) + p(x,t)$ at the right- and left-hand ends is

$$\begin{aligned} j_\rightarrow(t) &\equiv j(L,t) = \frac{\pi}{2L^2}\mathrm{e}^{\frac{(1-\alpha)L}{2}-\frac{t}{4}}\vartheta_3'\left(\frac{\pi[\alpha+1]}{2}, z(t)\right) \\ j_\leftarrow(t) &\equiv -j(0,t) = -\frac{\pi}{2L^2}\mathrm{e}^{-\frac{\alpha L}{2}-\frac{t}{4}}\vartheta_3'\left(\frac{\pi\alpha}{2}, z(t)\right). \end{aligned} \tag{3}$$

With the minus sign in its definition, $j_\leftarrow(t) \geqslant 0$.

The splitting probability, i.e. the probability that the particle is absorbed finally by the left- or the right-hand boundary, $n_\leftarrow = \int_0^\infty j_\leftarrow(t)\,\mathrm{d}t$ and $n_\rightarrow = \int_0^\infty j_\rightarrow(t)\,\mathrm{d}t$, and obviously $n_\leftarrow + n_\rightarrow = 1$. Using the integral formula

$$\int_0^\infty \mathrm{e}^{-as}\vartheta_3'\left(\left[\frac{x}{l}+1\right]\frac{\pi}{2}, \mathrm{e}^{-\frac{\pi^2}{l^2}s}\right)\mathrm{d}s = \frac{2l^2}{\pi}\frac{\sinh(x\sqrt{a})}{\sinh(l\sqrt{a})} \tag{4}$$

which holds for $|x| < l$ [16], we obtain

$$n_\leftarrow = \frac{\mathrm{e}^{-\alpha L} - \mathrm{e}^{-L}}{1-\mathrm{e}^{-L}} \qquad \text{and} \qquad n_\rightarrow = \frac{1-\mathrm{e}^{-\alpha L}}{1-\mathrm{e}^{-L}}. \tag{5}$$

Another important quantity is the *mean first-passage time*, i.e. the average time it takes for the particle to be absorbed by any of the boundaries. The probability distribution of this time is just the total probability current at the boundaries: $j_{\mathrm{out}} = j_\leftarrow + j_\rightarrow$. The mean first-passage time is then $\tau = \int_0^\infty t j_{\mathrm{out}}(t)\,\mathrm{d}t$. The calculation of τ is straightforward using the derivative of (4) w.r.t. a, and the result is

$$\tau = L(n_\rightarrow - \alpha). \tag{6}$$

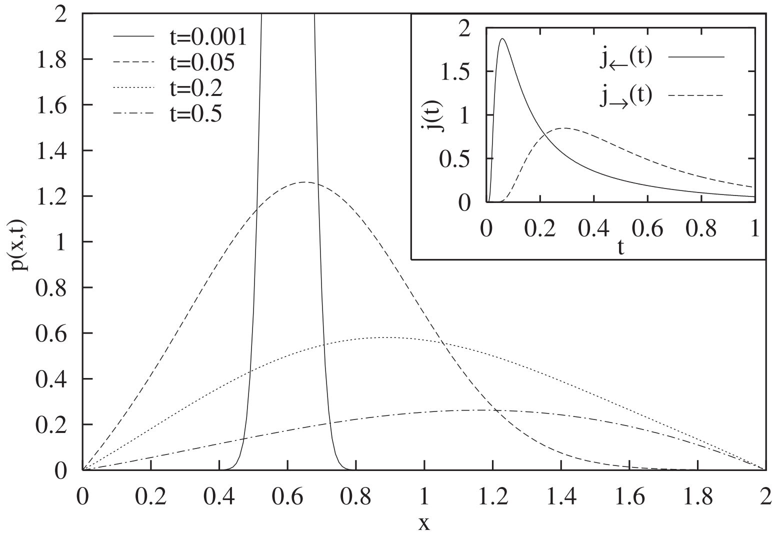

Figure 4. The time evolution of the probability distribution, when $L = 2$ and $\alpha = 0.3$. Note the difference between the probability distribution here and in figures 2 and 3, which is due to the different boundary condition. Inset: the probability current at the left- and right-hand boundaries.

There is another way to calculate $n_\rightarrow$ and τ, in which there is no need for an explicit formula for the time-dependent probability distribution or the current at the borders [2]. An ordinary differential equation can be written for $n_\rightarrow$, which, using our notation, is $-L\partial_\alpha n_\rightarrow + \partial_\alpha^2 n_\rightarrow = 0$ with boundary condition $n_\rightarrow|_{\alpha=0} = 0$ and $n_\rightarrow|_{\alpha=1} = 1$. By direct substitution one can verify that (5) is the solution. A similar equation can be written for the mean first-passage time: $-L\partial_\alpha \tau + \partial_\alpha^2 \tau = -L^2$ with boundary condition $\tau|_{\alpha=0} = 0$ and $\tau|_{\alpha=1} = 0$. It is easy to check that (6) is the solution for this equation.

3. Discussion of the results

First we summarize our results with dimensionalized parameters. The probability density is

$$p(x,t) = \frac{1}{2L} \mathrm{e}^{-\frac{v(2[\alpha L - x] + vt)}{4D}} \left\{ \vartheta_3\left(\left[\alpha - \frac{x}{L}\right]\frac{\pi}{2}, \tilde{z}(t) \right) - \vartheta_3\left(\left[\alpha + \frac{x}{L}\right]\frac{\pi}{2}, \tilde{z}(t) \right) \right\} \tag{7}$$

with the notation $\tilde{z}(t) \equiv \mathrm{e}^{-\pi^2 Dt/L^2}$. The currents at the right- and left-hand borders are

$$\begin{aligned} j_\rightarrow(t) &= \frac{\pi D}{2L^2} \mathrm{e}^{-\frac{v(2[\alpha-1]L+vt)}{4D}} \vartheta_3' \left(\frac{[\alpha-1]\pi}{2}, \tilde{z}(t) \right) \\ j_\leftarrow(t) &= -\frac{\pi D}{2L^2} \mathrm{e}^{-\frac{v(2\alpha L+vt)}{4D}} \vartheta_3' \left(\frac{\alpha\pi}{2}, \tilde{z}(t) \right). \end{aligned} \tag{8}$$

The splitting probability is $n_\rightarrow = \dfrac{1 - \mathrm{e}^{-\alpha L v/D}}{1 - \mathrm{e}^{-Lv/D}}$, and the mean first-passage time is $\tau = L(n_\rightarrow - \alpha)/v$. In the $v = 0$ case (7) and (8) are valid with $v = 0$ substitution, while for the splitting probability and the mean first-passage time we can take the $v \to 0$ limit and obtain $n_\rightarrow = \alpha$ and $\tau = \alpha(1-\alpha)L^2/(2D)$.

Since the splitting probability is the most important quantity as far as the segregation is concerned, we analyse it in detail. Its dependence on all four parameters v, D, α and L

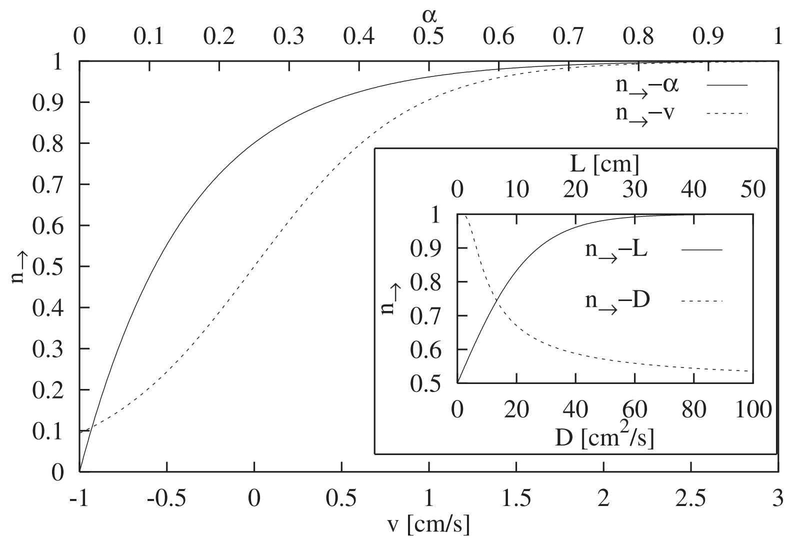

Figure 5. Dependence of the splitting probability $n_\rightarrow$ on all the parameters. The default values for the parameters are $v = 1.42$ cm s^{-1}, $D = 4.42$ cm s^{-1} (the fitted values in figure 2), $\alpha = 0.5$ and $L = 20$ cm.

can be seen in figure 5. It can be easily understood that with larger (positive) velocity or smaller diffusion constant the right arriving probability is closer to 1. It is also trivial that if the starting position is closer to the right-hand end then $n_\rightarrow$ is larger. However, to understand the dependence on the system width, we have to recall that in the case of drift-diffusion with natural boundary conditions (i.e. when the system is infinitely wide) the expectation value of the position is proportional to the time, while the dispersion is proportional only to the square root of time. Although this is not exactly true in the case of absorbing boundaries, the tendencies remain the same; therefore, in the case of $v > 0$, the larger the system width is, the lower the fraction of the probability that is absorbed by the left-hand boundary, and, as a consequence, the rest is absorbed by the right-hand boundary.

4. An application: segregation

As mentioned in the introduction, our motivation for the above calculations has been the application for segregating binary granular mixtures. For this purpose, now let us investigate the segregation properties of the system.

We begin with an illustrative example, the case of symmetric initial condition, $\alpha = 1/2$. Denoting v/D by u, the splitting probabilities are

$$n_\leftarrow = \frac{1}{1 + \mathrm{e}^{uL/2}} \qquad n_\rightarrow = \frac{1}{1 + \mathrm{e}^{-uL/2}}. \tag{9}$$

For definiteness, let us have a particle with $u > 0$, for example. For a small L, both probabilities are around $1/2$:

$$n_\leftarrow \approx 1/2 - uL/8 \qquad n_\rightarrow \approx 1/2 + uL/8. \tag{10}$$

For large L,

$$n_\leftarrow \approx \mathrm{e}^{-uL/2} \qquad n_\rightarrow \approx 1 - \mathrm{e}^{-uL/2}; \tag{11}$$

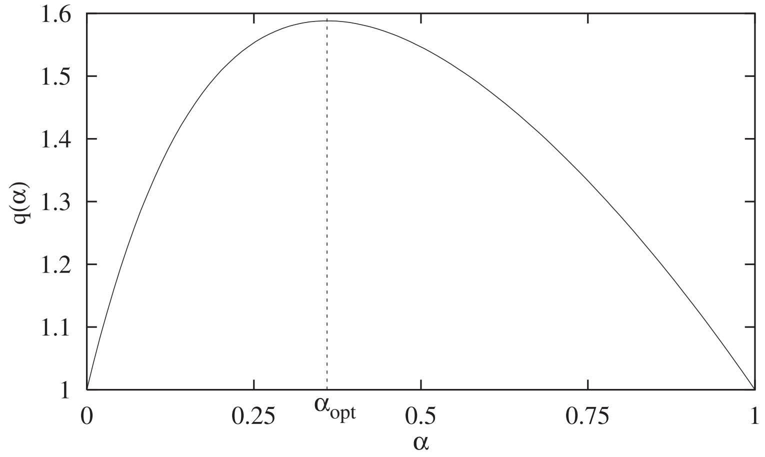

Figure 6. Dependence of q on α, for $u_1L = -1$ and $u_2L = 5$.

they tend to zero and one, respectively, in an exponential way in L. We can see that, for a small L, it is the diffusion, the left–right symmetric effect, that determines the left and right probabilities. On the other side, for large L, the drift becomes the dominating effect: it drives the particle to the direction of u with a probability that differs from 1 only by an exponentially small amount. This latter phenomenon makes it possible to use the system for segregation.

To study the segregation properties in more detail, now let us have two types of particles, with $u_1 < 0 < u_2$. We neglect the interaction between particles, which is a good approximation at low particle numbers. The expectation is that the particles with u_1 will tend to move to the left-hand end and the others to the right-hand end. Therefore, we can characterize the quality of the segregation with the quantity

$$q = n_{\leftarrow}(u_1) + n_{\rightarrow}(u_2). \tag{12}$$

Let us put the question of whether, for a given L, it is possible to choose an optimal α, i.e. where q is maximal[5].

Investigation of the function $q(\alpha)$ shows that it indeed has one maximum, at

$$\alpha_{\text{optimal}} = 1 - \frac{\ln \frac{u_1(\mathrm{e}^{u_2L}-1)}{u_2(\mathrm{e}^{u_1L}-1)}}{(u_2 - u_1)L}. \tag{13}$$

(For an illustration of the typical dependence of q on α, see figure 6.)

For practical purposes, we are interested in large L. In this asymptotic region, with the notation $\lambda = u_2/|u_1|$,

$$\alpha_{\text{optimal}} \approx \frac{1}{1+\lambda} + \frac{\ln\lambda}{1+\lambda}\,\frac{1}{|u_1|L} = \frac{1}{1+\lambda} + \mathcal{O}\left(\frac{1}{L}\right). \tag{14}$$

Consequently,

$$\begin{aligned} n_{\leftarrow}(u_1) &\approx 1 - c_1\mathrm{e}^{-\frac{\lambda}{1+\lambda}|u_1L|} \\ n_{\rightarrow}(u_2) &\approx 1 - c_2\mathrm{e}^{-\frac{1}{1+\lambda}|u_2L|} \end{aligned} \tag{15}$$

[5] Another natural choice to describe the quality of the segregation is $q' = n_{\leftarrow}(u_1)n_{\rightarrow}(u_2)$. Since the two functions, $q(\alpha)$ and $q'(\alpha)$, prove to differ only very slightly and lead to almost identical α_{optimal}, the two quantities are practically equivalent choices.

where $c_1 = \lambda^{\frac{1}{1+\lambda}}$ and $c_2 = \lambda^{\frac{-\lambda}{1+\lambda}}$. Therefore, we can see that, for large L, it is possible to choose such an optimal α that both segregation probabilities are exponentially close to 1 (as functions of L), the quality of the segregation is exponentially close to perfect.

5. Summary

We have presented a complete solution to the problem of one-dimensional drift-diffusion (with constant external force) between two absorbing boundaries: the probability distribution, the probability current at the boundaries (i.e. the rate of absorption), the splitting probability and the mean first-passage time were calculated. The results were applied to predict the quality of granular segregation in a vertically vibrated ratchet. We found that if the components have opposite drift velocities, the quality of the segregation of a binary mixture increases rapidly with increasing system width, and, as a limiting case, perfect segregation can be achieved. Furthermore, when the system width is fixed, we found the place where the granular mixture should be loaded into the system to obtain the best segregation quality.

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References

[1] Crank J 1975 *The Mathematics of Diffusion* (Oxford: Clarendon)
[2] Gardiner C W 1983 *Handbook of Stochastic Methods for Physics, Chemistry and the Natural Sciences* (Berlin: Springer)
[3] Risken H 1989 *The Fokker–Planck Equation* (Berlin: Springer)
[4] van Kampen N G 1992 *Stochastic Processes in Physics and Chemistry* (Amsterdam: North-Holland)
[5] Biswas P, Majumdar A, Mehta A and Bhattacharjee J K 1998 *Physica* A **248** 379
[6] Bustingorry S, Reyes E R and Cáceres M O 2000 *Phys. Rev.* E **62** 7664
[7] El-Shehawey M A 2000 *J. Phys. A: Math. Gen.* **33** 9005
[8] Luck J M and Mehta A 2000 *Preprint* cond.mat/0008400
[9] Rosato A, Strandburg K J, Prinz F and Swendsen R H 1987 *Phys. Rev. Lett.* **58** 1038
[10] Zik O, Levine D, Lipson S G, Shtrikman S and Stavans J 1994 *Phys. Rev. Lett.* **73** 644
[11] Makse H A, Havlin S, King P R and Stanley H E 1997 *Nature* **386** 379
[12] Lubachevsky B D 1991 *J. Comput. Phys.* **94** 255
[13] Walton O R 1992 *Particulate Two-Phase Flow* ed O M Roco (Boston: Butterworth–Heinemann)
[14] Farkas Z, Tegzes P, Vukics A and Vicsek T 1999 *Phys. Rev.* E **60** 7022
[15] Abramowitz M and Stegun I A 1965 *Handbook of Mathematical Fuctions* (New York: Dover) p 576
[16] Erdélyi A *et al* 1954 *Tables of Integral Transforms* vol 1 (New York: McGraw-Hill) p 224