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1990 J. Phys. A: Math. Gen. 23 L1169

(http://iopscience.iop.org/0305-4470/23/22/003)

J. Phys. A: Math. Gen. 23 (1990) L1169–L1173. Printed in the UK

LETTER TO THE EDITOR

Nearest-neighbour distances of diffusing particles from a single trap

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Received 14 September 1990

Abstract. We present a simple method for obtaining the typical smallest distance from an absorbing trap to the nearest particle in a system of Brownian particles. In terms of the overall density profile, we also obtain the distribution function for the minimum distance. By using a quasistatic approximation for the diffusion equation, we derive new results for two dimensions: the characteristic distance to the nearest particle increases asymptotically as $\sqrt{\ln(t)}$. The technique is useful in diffusion–reaction systems.

In the Smoluchowski model for bimolecular reactions, an ideal spherical trap centred at the origin is surrounded by a cloud of Brownian particles which are captured upon contact with the trap. The reaction rate in this formulation depends on the spatial distribution of particles about the trap. Recently, interest has focused on finer details of this distribution such as the distance of the nearest surviving particle from the trap [1–3]. The density distribution function of that distance is the key to several exact results concerning some diffusion–reaction systems in one dimension [4].

While the spatial density of the particles surrounding the trap can be easily obtained by solving a diffusion equation with the appropriate boundary conditions, the distance to the nearest particle from the trap seems to require a more sophisticated analysis [1]. In this paper, we suggest a simple derivation for the typical distance from the trap to the nearest particle and of the distribution of those distances, based upon the more readily attainable spatial density of all particles and simple facts from the statistics of extremes [5, 6]. To demonstrate our method, we rederive the known results for one and three dimensions. The simplicity of our approach, together with using a quasistatic approximation [7] for solving the diffusion equation, allows us to solve the two-dimensional case for the first time.

Consider first the one-dimensional problem: a perfect trap is located at the origin and is initially surrounded by a homogeneous density, c_0, of Brownian particles which diffuse with a diffusion constant D. The density $c(x, t)$ of the surviving particles (to the right of the trap) is given by the diffusion equation

$$\frac{\partial}{\partial t} c(x, t) = D \frac{\partial^2}{\partial x^2} c(x, t) \qquad x \geqslant 0 \tag{1a}$$

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0305-4470/90/221169+05$03.50

with the initial and boundary conditions

$$c(x, 0) = c_0 \tag{1b}$$

$$c(0, t) = 0. \tag{1c}$$

The solution to (1*a*)-(1*c*) is

$$c(x, t) = c_0 \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) \tag{2}$$

where $\operatorname{erf}(z) = (2/\sqrt{\pi}) \int_0^z \exp(-u^2)\, du$ is the error function.

To compute $x_{\min}$, a characteristic minimum distance from the surviving particle which is closest to the trap, we observe that the criterion

$$\int_0^{x_{\min}} c(x, t)\, dx = 1 \tag{3}$$

specifies that there will be one particle which is a distance $x_{\min}$ or less from the trap. Thus, we identify $x_{\min}$ as the typical distance from the trap to the nearest particle. Using the expression for $c(x, t)$ from (2) in (3) yields, in the long-time asymptotic limit

$$x_{\min} = 2^{3/4} \pi^{1/4} \left(\frac{Dt}{c_0^2}\right)^{1/4}. \tag{4}$$

Next, we compute $p(x, t)$, the probability density function for $x_{\min}$. To this end we first derive an expression for the probability that the nearest particle to the trap is at a distance equal or larger than x. Let $N(y, t) = \int_0^y c(x, t)\, dx$ be the expected number of surviving particles in the interval $(0, y)$, where $y \gg x$. The probability that a single particle is not in the interval $(0, x)$ is simply $1 - N(x, t)/N(y, t)$. Hence, the probability, $P(x, t)$, that no particles are inside the interval $(0, x)$ equals $(1 - N(x, t)/N(y, t))^{N(y, t)}$. Since $N(x, t) \ll N(y, t)$ we can approximate $P(x, t)$ as $\exp(-\int_0^x c(x', t)\, dx')$. Finally, $p(x, t) = -\partial P(x, t)/\partial x$, leading to

$$p(x, t) = c(x, t) \exp\left(-\int_0^x c(x', t)\, dx'\right). \tag{5}$$

Equation (5) is of course valid only in the long-time asymptotic limit. Substituting the $t \to \infty$ limit of $c(x, t)$ given in (2) into (5), we find

$$p(x, t) = \frac{c_0 x}{\sqrt{\pi D t}} \exp\left(\frac{-c_0 x^2}{2\sqrt{\pi D t}}\right). \tag{6}$$

This is the result for the (one-sided) distance distribution found by Weiss *et al* in one dimension [1]. Notice that $x_{\min}$ computed by (3) is not equal to the average distance of the nearest surviving particle from the trap that arises from (6), though the two quantities scale in the same manner.

An even easier way to derive the functional form of $p(x, t)$ and $x_{\min}$ is by employing a quasistatic approximation to solve the diffusion equation. In this approximation the explicit time derivative in the diffusion equation is neglected and the time dependence in the equation is accounted for by a moving boundary condition [7]. This very simple approach is found to work remarkably well in a variety of physical situations. For the trapping problem in one dimension, we solve the static diffusion (Laplace) equation in the 'active' region $x < \sqrt{Dt}$, subject to the boundary condition that at $x^* = \sqrt{Dt}$ the solution from the Laplace equation must equal c_0. The solution to $0 = D\partial^2 c/\partial x^2$ for

$x \ll \sqrt{Dt}$ is $c = \text{constant} \times x$ (this satisfies the boundary condition (1c)), and for $x \gg \sqrt{Dt}$ we take $c = c_0$ (this satisfies the initial condition (1b)). Extending and matching these functions at x^* one obtains the approximation

$$c(x,t) \approx \begin{cases} c_0 x/\sqrt{Dt} & x < \sqrt{Dt} \\ c_0 & x > \sqrt{Dt}. \end{cases} \tag{7}$$

Using this form of $c(x, t)$ for $x \ll \sqrt{Dt}$ in (3) and (5) leads to the correct functional forms of $x_{\min}$ and $p(x, t)$ in one dimension. The essential point here is that for the minimum distance we require the density distribution only for very small x, and this is obtained exactly in the quasistatic approximation.

Consider next the Smoluchowski problem in three dimensions. The trap must now have a finite dimension to make trapping possible. Let the trap be a sphere of radius a, centred at the origin. The diffusion equation is

$$\frac{\partial}{\partial t} c(r,t) = D \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} c(r,t) \qquad r \geq a \tag{8a}$$

with the initial and boundary conditions

$$c(r,0) = c_0 \qquad r \geq a \tag{8b}$$

$$c(a,t) = 0. \tag{8c}$$

Although an exact solution can be obtained straightforwardly, we use the quasistatic approximation and then derive the functional form of $r_{\min}$ and $p(r, t)$. The solution of the static equation for $a \leq r \ll \sqrt{Dt}$ is $c = \text{constant} \times (1/a - 1/r)$, and $c = c_0$ for $r \gg \sqrt{Dt}$. Matching the solutions at $r^* = \sqrt{Dt}$ fixes the value of the constant to $c_0\sqrt{Dt}/(\sqrt{Dt} - a)$, so that in the long-time asymptotic limit one has

$$c(r,t) = c_0\left(1 + \frac{a}{\sqrt{Dt}}\right)\left(1 - \frac{a}{r}\right) \qquad a \leq r \ll \sqrt{Dt}. \tag{9}$$

Notice that, in fact, $c(r, t)$ becomes independent of time as $t \to \infty$, and agrees with the exact solution to (8). Since the limit $c(r, t \to \infty)$ exists, $r_{\min} \to$ constant. Using (5) we find

$$p(r,t) = 4\pi r^2 c_0\left(1 + \frac{a}{\sqrt{Dt}}\right) \exp\left[-4\pi r^2 c_0\left(1 + \frac{a}{\sqrt{Dt}}\right)\left(\frac{\rho^3 - 1}{3} - \frac{\rho^2 - 1}{2}\right)\right] \tag{10}$$

where $\rho = r/a$ and the factors of $4\pi r^2$ occur because in three dimensions $N(r) = \int_a^r 4\pi r^2 c(r,t)\,\mathrm{d}r$. The result in (10) is identical to that of Weiss *et al* [1].

Finally, we address the Smoluchowski problem in two dimensions. Assuming, once more, a trap of radius a, the diffusion equation is

$$\frac{\partial}{\partial t} c(r,t) = D \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} c(r,t) \qquad r \geq a \tag{11a}$$

$$c(r,0) = c_0 \qquad r \geq a \tag{11b}$$

$$c(a,t) = 0. \tag{11c}$$

The quasistatic approximation now yields

$$c(r,t) = \frac{c_0}{\ln(\sqrt{Dt}/a)} \ln(r/a) \qquad a \leq r \ll \sqrt{Dt}. \tag{12}$$

To compute $r_{\min}$, we use $\int_a^{r_{\min}} 2\pi r c(r, t)\, dr = 1$. Then $\rho_{\min} = r_{\min}/a$ is obtained as the solution to the transcendental equation

$$\rho^2 \ln \rho - \tfrac{1}{2}(\rho^2 - 1) = (\tfrac{1}{2}\pi c_0 a^2) \ln(Dt/a^2). \tag{13}$$

The numerical solution of (13) is plotted in figure 1. For $t \to \infty$, $r_{\min} \sim \sqrt{\ln(Dt/a^2)/2\pi c_0}$. Finally, the long-time asymptotic limit of the distribution function for the distance of the nearest particle is

$$p(r, t) = \frac{2\pi c_0 a}{\ln(\sqrt{Dt}/a)} \rho \ln \rho \exp\left[-\frac{2\pi c_0 a}{\ln(\sqrt{Dt}/a)} \left(\frac{\rho^2}{2} \ln \rho - \frac{\rho^2 - 1}{4} \right) \right]. \tag{14}$$

In summary, by basic notions of extreme statistics there exists a straightforward relation between the form of the density profile of Brownian particles near a trap, $c(x, t)$, the characteristic distance of the nearest surviving particle, $x_{\min}$, and the probability density function of that distance, $p(x, t)$. Equations (3) and (5) express these relations in one dimension. The generalization of these equations to higher dimensions is trivial. Furthermore, because we are interested only in the long time asymptotic limit, it is possible to employ a simplifying quasistatic approximation for the diffusion equation, whereby the explicit time dependence is dropped and is reintroduced through a moving boundary condition. We have illustrated the method by rederiving known results in dimensions one and three, and have exploited the simplicity of the approximation to obtain the solution in the borderline case of two dimensions. In two dimensions, the distance of the nearest particle to the trap increases as $\sqrt{\ln(t)}$.

We notice that the relations between $c(x, t)$, $x_{\min}$, and $p(x, t)$ can be applied to other related problems. For example, Schoonover *et al* [3] have studied a version of the one-dimensional Smoluchowski problem where in addition to the particles the trap is also allowed to diffuse with a diffusion constant D_T. They find that $x_{\min} \sim t^{\alpha}$, where α is a smoothly varying function of the ratio $\Delta = D_T/D$, increasing from $\alpha = 1/4$ for $\Delta = 0$ to $\alpha = 1/2$ for $\Delta = \infty$. Using (3) and the scaling assumption $c(x, t) = f(x/\sqrt{t})$, one can show that $c(x, t) \sim (x/\sqrt{t})^{2\alpha/(1-2\alpha)}$ in the long-time asymptotic limit. Then using (5), one would get $p(x, t) \sim (x/\sqrt{t})^{2\alpha/(1-2\alpha)} \exp[-\text{constant} \times (x/t^{\alpha})^{1/(1-2\alpha)}]$.

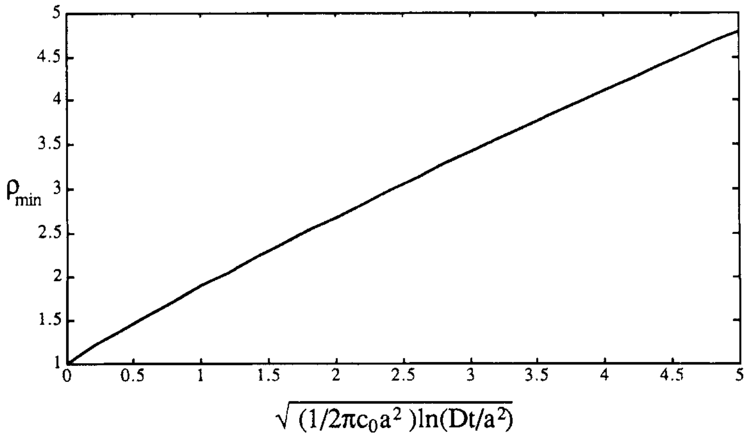

Figure 1. Plot of the numerical solution to (13), the typical distance of the nearest particle to the trap in two dimensions.

The authors wish to thank the US Army Research Office and the Donors of the Petroleum Research Foundation for partial support of this work. We also thank H Reiss for helpful advice and formulae about [7].

Note added in proof. After this manuscript was completed we learned of closely related work by Havlin *et al* in which the nearest-neighbour distance distribution in two dimensions is derived by independent means. We are grateful to S Havlin for informing us of these results before publication.

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