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TOPICS IN BROWNIAN MOTION WITH APPLICATION IN BIOPHYSICS

by

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ABSTRACT

In this thesis, we studied some properties of Brownian motion and application in the medical area.

In Chapters II and III, the two–dimensional Brownian motion of circular disks is considered where these join to form groups whenever they touch. The total number of groups N_t is considered as a function of time. An upper bound for N_t^{-1} is derived and compared to the experimental movement of erythrocytes (red blood cells). Cells at pH = 7.4 and pH = 6.3 are shown to have a group count that respectively exceeds and falls below the plotted bound. This provides evidence that live cells have a tendency to coalesce that is not explained by Brownian motion only.

In Chapter IV, points executing free Brownian motion are randomly placed in the region $b < r \leq a$ of $\mathbb{R}^n$. The distribution of first hitting time on the central stationary n–sphere is derived. For $n = 3$, the moment generating function of the first hitting time is derived.

In Chapter V, a Brownian particle is selected at random from a region E in $\mathbb{R}^n$ and then the probability that the particle will be in a convex region G in $\mathbb{R}^n$ a time t later, where $E \subset G$, is derived. The probabilities for (a) $E = G$, disc or ball and (b) $E \subset G$, concentric spheres are calculated.

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Dedicated to my parents

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CHAPTER I

INTRODUCTION

1.1 HISTORICAL BACKGROUND

Robert Brown was a distinguished botanist. Although Brown is remembered by mathematicians only as the discoverer of Brownian motion, his biography in the Encyclopedia Britannica makes no mention of this discovery.

In the early eighteenth century, Brown was studying the fertilization process in several different species of flower. Looking at the pollen in water through a microscope, he observed small particles in "rapid oscillatory motion".

Of the causes of Brownian motion, Brown [1829] writes:

"I have formerly stated my belief that these motions of the particles neither arose from currents in the fluid containing them, nor depended on that intestine motion which may be supposed to accompany its evaporation.

These causes of motion, however, either singly or combined with other, –as, the attractions and repulsions among the particles themselves, their unstable equilibrium in the fluid in which they are suspended, their hygrometrical or capillary action, and in some cases the disengagement of volatile matter, or of minute air bubbles, –have been considered by several writers as sufficiently accounting for the appearances."

His theory, is that matter is composed of small particles, which exhibit a rapid, irregular motion having its origin in the particles themselves and not in the surrounding fluid.

His contribution was to demonstrate the presence of Brownian motion in inorganic as well as organic matter and establish it's importance.

The first to express a notion close to the modern theory of Brownian motion was Wiener in 1863.

During 1850 – 1900, many scientists worked on the phenomenon. The following main points were noted:

a. The motion is very irregular, composed of translations and rotations, and the trajectory appears to have no tangent.

b. Two particles appear to move independently.

c. The activity of the motion is directly proportional to the temperature, and inversely proportional to the viscosity of the fluid and size of the particles.

d. The motion never ceases.

In 1905, Albert Einstein formulated a correct quantitative theory of Brownian motion. There are two parts to Einstein's argument. The first is mathematical. The result is the following:

Let $p = p_t(x_1, x_2, x_3)$ be the probability density of a Brownian particle at the point (x_1, x_2, x_3) at time t. Then, Einstein derived the diffusion equation

$$\frac{\partial p}{\partial t} = D\nabla^2 p$$

where D is a positive constant,

and ∇^2 is the Laplacian operator.

If the particle is at the origin 0 at time 0, then

$$p_t(x_1, x_2, x_3) = \frac{1}{(4\pi Dt)^{3/2}}\, e^{-\frac{(x_1^2 + x_2^2 + x_3^2)}{4Dt}} .$$

The second part of his argument, which relates D to other physical quantities, is physical.

If the Brownian particles are spheres of radius a, then combined with Stokes' theory of friction, we have the Stokes–Einstein relation:

$$D = \frac{KT}{6\pi \eta a}$$

where T is the absolute temperature,

η is the coefficient of viscosity

and K is the Boltzmann's constant.

A mathematical theory of the behaviour of coagulating particles undergoing Brownian motion in three dimensions was first given by Smoluchowski (1916) and later elaborated by Chadrasekhar (1943). Other formulations of coagulation and reaction based upon diffusion (Noyes, 1961; Waite, 1957; Collins & Kimble, 1949) are essentially identical to those of Smoluchowski. Treatment of the problem in a finite two–dimensional medium (Owens, 1974; Adam & Delbruck, 1968; Razi Naqvi, 1974) has been largely motivated by considerations of movement of molecules on lipid membranes. (See Eldridge 1980)

1.2 BASIC DEFINITION & FORMULAE

The following definitions (1.2.1, 1.2.2) are quoted from Karlin and Taylor (1974).

1.2.1 ONE DIMENSIONAL BROWNIAN MOTION

Brownian motion is a stochastic process $\{X(t);\ t \geq 0\}$ with the following properties:

(a) Every increment $X(t+s) - X(s)$ is normally distributed with mean 0 and variance $\sigma^2 t$; σ is a fixed parameter.

(b) For every pair of disjoint time intervals $[t_1, t_2]$, $[t_3, t_4]$, the increments $X(t_4) - X(t_3)$ and $X(t_2) - X(t_1)$ are independent random variables with distributions given in (a), and similarly for n disjoint time intervals where n is an arbitrary positive integer.

(c) $X(0) = 0$ and $X(t)$ is continuous at $t = 0$.

This means that we postulate that a displacement $X(t+s) - X(s)$ is independent of the past, or alternatively, if we know $X(s) = x_0$, then no further knowledge of the values of $X(\tau)$, for $\tau < s$ has any effect on our knowledge of the probability law governing $X(t+s) - X(s)$. Written formally, this says that if $t > t_0 > t_1 > \cdots > t_n$,

$$P\left\{X(t) \le x \mid X(t_0) = x_0, X(t_1) = x_1, \cdots, X(t_n) = x_n\right\}$$
$$= P\left\{X(t \le x) \mid X(t_0) = x_0\right\}$$

This is a statement of the Markov character of the process.

Under the condition that $X(0) = 0$, the variance of $X(t)$ is σ^2 t. Hence σ^2 is sometimes called the variance parameter of the process. The process $\tilde{X}(t) = \frac{X(t)}{\sigma}$ is a Brownian motion process having variance parameter of one, called standard Brownian motion. By this device we may always reduce an arbitrary Brownian motion to a standard Brownian motion.

By part (a) of the definition with $\sigma^2 = 1$, we have

$$P\left\{X(t) \le x \mid X(t_0) = x_0\right\} = P\left\{X(t) - X(t_0) \le x - x_0\right\}$$

$$= \frac{1}{\sqrt{2\pi(t-t_0)}} \int_{-\infty}^{x-x_0} \exp\left[-\frac{\alpha^2}{2(t-t_0)}\right] d\alpha.$$

The consistency of part (b) of the definition with part (a) follows from well-known properties of the normal distribution,

e.g. if $t_1 \le t_2 \le t_3$ then

$$X(t_3) - X(t_1) = [X(t_3) - X(t_2)] + [X(t_2) - X(t_1)].$$

On the right we have independent normal random variables with mean 0 and variances $t_3 - t_2$ and $t_2 - t_1$, respectively. Hence their sum is normal with mean 0 and variance $t_3 - t_1$ as it should be.

1.2.2 MULTIDIMENSIONAL BROWNIAN MOTION

Let $\{X_1(t);\ t \ge 0\}$, $\cdots$ $\{X_N(t);\ t \ge 0\}$ be standard Brownian motion processes, statistically independent of one another. The vector-valued process defined by

$$X(t) = \left[X_1(t), \cdots, X_N(t)\right]$$

is called N-dimensional Brownian motion. The motion of a particle undergoing Brownian motion in the plane and in space are described by two-dimensional and three-dimensional Brownian motions, respectively.

If the particle is at the origin 0 at time 0, let $p_t(x_1, x_2, \ldots, x_n)$ be the probability density of a particle reaches the point $(x_1, x_2, \ldots, x_n)$ at time t, then

$$p_t(x_1, x_2, \ldots, x_n) = \frac{1}{(2\pi t)^{n/2}}\, e^{-\frac{(x_1^2 + \cdots + x_n^2)}{2t}}.$$

1.3 RADIAL BROWNIAN MOTION

Let $\{X(t): \ t \geq 0\}$ be an N–dimensional Brownian motion process. The stochastic process defined by

$$R(t) = \left[X_1(t)^2 + \cdots + X_N(t)^2\right]^{\frac{1}{2}}, \qquad t \geq 0$$

is called Radial Brownian motion or the Bessel process with parameter $\frac{1}{2}$ N–1. It is a Markov process having continuous sample paths in the state space $[0, \infty)$ (see Karlin and Taylor (1974) page 368).

The probability transition density of the N–dimensional process from r_1 to r_2 in a time t is given by (Kent equation 9.1).

$$p_t(r_1, r_2) = t^{-1} r_1^{-\nu} I_\nu\left[\frac{r_1 r_2}{t}\right] \exp\left[-\frac{1}{2t}(r_1^2 + r_2^2)\right] r_2^{\nu+1}$$

$$t > 0,\ r_1,\ r_2 > 0 \qquad (1.3.1)$$

where $\nu = (N-2)/2 > -1$ and

$I_\nu(x)$ is the modified Bessel function of the first kind

$$I_\nu(x) = \sum_{k=0}^{\infty} \frac{\left[\frac{x}{2}\right]^{2k+\nu}}{k!\,\Gamma(k+\nu+1)}.$$

For N = 1, $I_{-\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}} \cosh x$,

$$p_t(r_1, r_2) = \sqrt{\frac{2}{\pi t}} \exp\left\{-\frac{r_1^2 + r_2^2}{2t}\right\} \cosh\left[\frac{r_1 r_2}{t}\right]. \qquad (1.3.2)$$

For N = 2,

$$p_t(r_1, r_2) = t^{-1} r_2 I_0\left[\frac{r_1 r_2}{t}\right] \exp\left[-\frac{1}{2t}(r_1^2 + r_2^2)\right]. \qquad (1.3.3)$$

For N = 3, $I_{\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}} \sinh x$

$$p_t(r_1, r_2) = \sqrt{\frac{2}{\pi t}} \exp\left\{-\frac{r_1^2+r_2^2}{2t}\right\} \frac{r_2}{r_1} \sinh\left[\frac{r_1 r_2}{t}\right]. \qquad (1.3.4)$$

By continuity of sample path, we have

$$p_t(0, r_2) = \lim_{r_1 \to 0} p_t(r_1, r_2).$$

Therefore for

(a) $N = 1,\ p_t(0, r_2) = \sqrt{\frac{2}{\pi t}} \exp\left\{-\frac{r_2^2}{2t}\right\}$

(b) $N = 2,\ p_t(0, r_2) = \frac{r_2}{t} \exp\left\{-\frac{r_2^2}{2t}\right\}$ (compare with eqn. 5.2.3)

(c) $N = 3,\ p_t(0, r_2) = \sqrt{\frac{2}{\pi t^3}}\, r_2^2 \exp\left\{-\frac{r_2^2}{2t}\right\}.$ (compare with eqn. 5.2.3)

1.4 ORIENTATION OF THE RESEARCH PROBLEM

In 1981, Rowlands and co–workers ([26], [27]) studied the aggregation of human red blood cells (erythrocytes). Aggregation indicates the existence of a long range attractive force between erythrocytes of a given species. Initially, at time t = 0, single disks are presented. From then onwards, they combine to form double, triple, ... i–fold disks. The clustering of erythrocytes is referred as rouleaux formation. They adopted Swift and Friedlander's (1964) simplifying assumption that all particles have the same radius (and the implication that all zones of attraction have the same radius $Z \neq r$). If N is the total number of particles (single and multiple) the kinetics of coagulation are governed by

$$\frac{1}{N_t} - \frac{1}{N_0} = \frac{4KT}{3\eta} \frac{Z}{r} t \qquad (1.4.1)$$

where k : Boltzman's constant

T : absolute temperature

η : viscosity of suspending medium

and r : radius of the particle

Equation 1.4.1 is for a three–dimensional process. Cells sediment, however, so the process is compressed into two dimensions and the rate constant will be higher by a factor of 1.5. Equation 1.4.1 becomes

$$\frac{1}{N_t} - \frac{1}{N_0} = \frac{2KT}{\eta} \frac{Z}{r} t$$

which predicts a linear relation between N_t^{-1} and t.

In an experiment, for a given t, one can count the number of cell groups (i.e. N_t). The regression of N_t^{-1} on t was computed.

An interaction coefficient Ξ is defined by $\frac{Z}{r}$.

If $\Xi = 1$, then it indicates a pure Brownian motion.

If $\Xi > 1$, then it indicates a zone of attraction.

If $\Xi < 1$, then it indicates a repulsive force.

In the experimental studies, Rowlands et al (1981, 1982) have observed values of Ξ up to approximately three indicating a long range attractive force between normal cells.

The assumptions of Rowlands and associates are:

1. $r_i = r_j$ for all i, j
2. $D_i = D_j$ for all i, j

   where r_i is the radius of i–fold disks

   and D_i is the diffusion coefficient of i–fold disks
3. $t >> \frac{r^2}{D}$.

We try to minimize the above assumption to find an upper bound of N_t^{-1}. Chapters II and III are based on the article that we published (Enns, Fung, Rowlands & Sewchand) in Cell Biophysics 5 (1983), p189–195.

1.5 METHODS OF GEOMETRIC PROBABILITY

Some new results in Brownian motion are attainable via methods of geometrical probability. In particular if one is viewing a cell undergoing Brownian motion under a microscope, it may be of interest whether this cell will still be in the viewing field at a time t later. This requires a knowledge of the distribution of the lengths of random rays under ν–radomness, the derivation of which follows.

Enns and Ehlers (1978, 1980, 1981, 1988) in a series of papers have derived the distributions of the lengths of random rays and secants under various randomness assumptions. We will provide the background derivations necessary for the new work in the thesis.

ν–randomness is defined as selecting a point P at random from a body K and also picking a random direction θ. In n–dimensions, the direction θ will be uniformly distributed in $[0, nC_n]$ where C_n is the volume of a unit n–sphere. One can now define a ray S of length ℓ as the distance from P to the boundary of K in direction θ. We will assume that K is a convex body in $\mathbb{R}^n$. A secant of length L will be formed by projecting the ray backwards to the surface of K. L will not be used, so we will only concentrate on the ray. Now if the body K is translated a distance ℓ in direction θ, then denote the translated K by $K(\ell,\theta)$. If one now places a needle of length ℓ in body K in direction θ, then the tip of the needle must lie in $K \cap K(\ell,\theta)$ for the whole needle to lie within K.

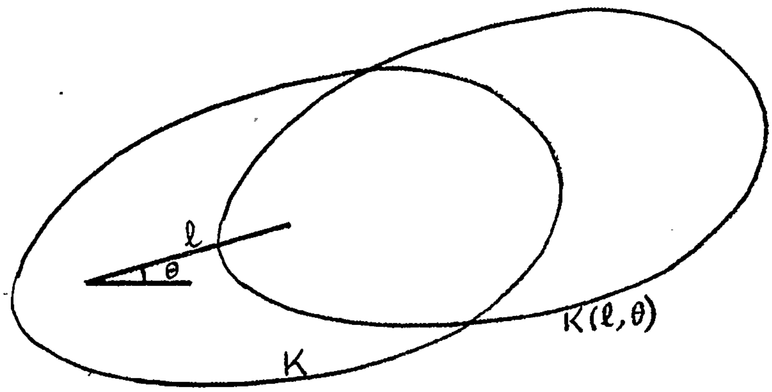


Figure 1.1

Now since the point P is chosen randomly in K, it must lie in $K \cap K(-\ell,\theta)$ for the ray R to be of length greater than ℓ. Therefore:

$$P(S > \ell | \theta) = \frac{V[K \cap K(-\ell,\theta)]}{V(K)}$$

$$= \frac{V[K \cap K(\ell,\theta)]}{V(K)}$$

where $V(\cdot)$ is the volume of $(\cdot)$. Averaging over θ, one obtains:

$$P(S > \ell) = \frac{\mathscr{E}_\theta[V(K \cap K(\ell,\theta)]}{V(K)}$$

$$= \Omega(\ell). \qquad (1.5.1)$$

This defines the normalized overlap function $\Omega(\ell)$. All other distributions derived in Enns and Ehlers (1978, 1980, 1981, 1988) are in terms of $\Omega(\ell)$ and its counterpart $\omega(\ell)$, which is the normalized overlap surface content of $K \cap K(\ell,\theta)$ when averaged over θ.

Equation (1.5.1) illustrates $\Omega(\ell)$ as an average over θ. However, since there are two random variables involved in generating R we can also express $\Omega(\ell)$ as an average over the randomly chosen point P.

Select a point P randomly in K and surround it with an n–sphere of radius ℓ.

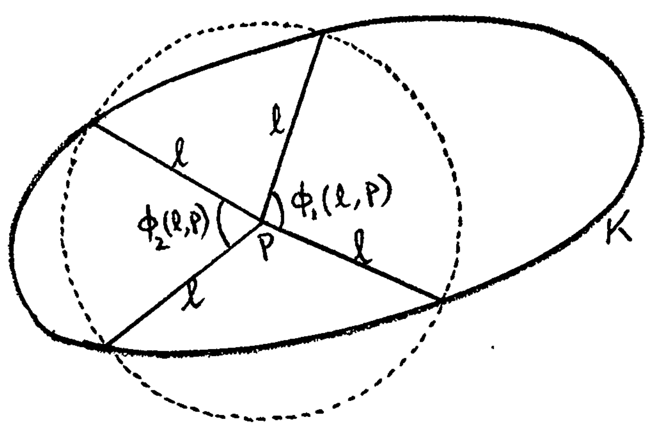


Figure 1.2

Define the solid angles subtended by the body K as $\phi_1(\ell,P)$ and $\phi_2(\ell,P)$. There may be zero, one or two such angles. Let $\phi(\ell,P) = \sum_i \phi_i(\ell,P)$ be the sum of these internal angles. Then

$$P(S > \ell | P) = \frac{\phi(\ell,P)}{nC_n} . \tag{1.5.2}$$

Equations (1.5.1) and (1.5.2) therefore relate the two averaging procedures. This will be the starting point of our derivation in Chapter V.

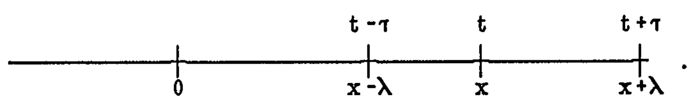
CHAPTER II

COAGULATIONS OF COLLOIDAL PARTICLES UNDER BROWNIAN MOTION

2.1 INTRODUCTION:

Smoluchowski (1917) succeeded in applying the principles of Brownian motion to describe the coagulations of colloidal particles due to the introduction of an electrolytic solution. Smoluchowski's theory is based on the view that around each discharged particle is a sphere of attraction such that if two particles undergoing Brownian motion enter each other's sphere, they adhere and never separate again. In his outset, a particle assumed fixed in space with a sphere of influence of radius b, is in a medium of infinite extent in which a number of Brownian particles of zero radius (regarded as points) are randomly scattered at time t = 0. Suppose that the stationary particle is at the origin of our system of coordinates and also assumed that when a point touches the boundary of the sphere, it will merge to the origin immediately.

The point of departure for the theory of diffusion is the random walk. Let us consider the one-dimensional space. Each individual moves a short distance λ to the right or left in a short time τ. We define the probability that a particle released from the origin at t = 0 reaches point x by time t to be p(x,t).



At one time interval earlier, i.e. at time $t-\tau$, the particle is at either of points $x-\lambda$ or $x+\lambda$. if we call α the probability that a particle will move to the right in time unit τ, and β the probability that the particle will move to the left $(\alpha+\beta = 1)$,

$$p(x,t) = \alpha\, p(x-\lambda,\ t-\tau) + \beta\, p(x+\lambda,\ t-\tau). \qquad (2.1.1)$$

To obtain a diffusion equation from (2.1.1), it is assumed that λ and τ are very small compared to x and t, respectively, and that each term on the right hand side of the equation (2.1.1) can be expanded in a Taylor series in x and t,

$$p(x-\lambda,t-\tau) = p(x,t) - \lambda \frac{\partial p}{\partial x} - \tau \frac{\partial p}{\partial t} + \frac{\lambda^2}{2} \frac{\partial^2 p}{\partial x^2} + \lambda\tau \frac{\partial^2 p}{\partial x \partial t} + \frac{\tau^2}{2} \frac{\partial^2 p}{\partial t^2}$$

$$. \qquad (2.1.2)$$

$$p(x+\lambda,t+\tau) = p(x,t) + \lambda \frac{\partial p}{\partial x} - \tau \frac{\partial p}{\partial t} + \frac{\lambda^2}{2} \frac{\partial^2 p}{\partial x^2} - \lambda\tau \frac{\partial^2 p}{\partial x \partial t} + \frac{\tau^2}{2} \frac{\partial^2 p}{\partial t^2}$$

All of the right–hand derivatives are evaluated at (x,t). If (2.1.2) is substituted into (2.1.1) and the relations $\alpha+\beta = 1$, $\alpha-\beta = \varepsilon$ are used, we have

$$\frac{\partial p}{\partial t} = -\frac{\lambda\varepsilon}{\tau} \frac{\partial p}{\partial x} + \frac{\lambda^2}{2\tau} \frac{\partial^2 p}{\partial x^2} + \lambda\varepsilon \frac{\partial^2 p}{\partial x \partial t} + \frac{\tau}{2} \frac{\partial^2 p}{\partial t^2} \qquad (2.1.3)$$

where the parameters λ, τ, and ε are assumed to be constant.

Now let us consider the limit as these parameters go to zero. We shall not do this indiscriminately; rather we shall suppose that as τ becomes small, λ and ε decrease so as to be of the same order of magnitude of $\tau^{\frac{1}{2}}$. In other words, in the first and second terms on the right–hand side of (2.1.3),

$$\lim_{\lambda,\varepsilon,\tau\to 0} \frac{\lambda\varepsilon}{\tau} = \mu, \quad \lim_{\lambda,\tau\to 0} \frac{\lambda^2}{2\tau} = D\ . \qquad (2.1.4)$$

Since the other right–hand terms converge to zero, the following equation is obtained,

$$\frac{\partial p}{\partial t} = - \mu \frac{\partial p}{\partial x} + D \frac{\partial^2 p}{\partial x^2} . \qquad (2.1.5)$$

This is the equation of diffusion for the random walk that results from the limiting process. If p in (2.1.5) is multiplied by the total number of particles in the system, the particle concentration W is obtain so that

$$\frac{\partial W}{\partial t} = - \mu \frac{\partial W}{\partial x} + D \frac{\partial^2 W}{\partial x^2} . \qquad (2.1.6)$$

For simple random walk case (by taking limit it will become Brownian motion), $\mu = 0$ since $\alpha - \beta = 0$, hence (2.1.6) can be written as

$$\frac{\partial W}{\partial t} = D \frac{\partial^2 W}{\partial x^2} . \qquad (2.1.7)$$

In two dimensions with horizontal and vertical displacements parallel to the x– and y– axis, we have

$$\frac{\partial W}{\partial t} = D\left[\frac{\partial^2 W}{\partial x^2} + \frac{\partial^2 W}{\partial y^2}\right] = D\nabla^2 W.$$

We have therefore to seek a solution of the diffusion equation:

$$\frac{\partial W}{\partial t} = D\nabla^2 W \qquad (2.1.8)$$

The problem that we are going to solve here is dealing with two–dimensional Brownian Motion which can be summarized as follows:

Consider an array of uniform circular disks of radius b whose motion is totally governed by Brownian movement. We assume the disks to be totally noninteracting, except on contact, in which case, they adhere, forming a doublet. When an i–fold disk touches with a j–fold disk, they form a k–fold disk where $k = i+j$. We will concentrate on the total number of disk groups N_t present per unit area as a function of time t. An upper bound for N_t^{-1} when only Brownian movement is present will be derived. If in an experiment, this upper bound is exceeded then we can conclude that there is evidence of a force of attraction among the disk groups of different sizes.

The approach to solving this problem basically follows Smoluchowski's. However due to the different dimension and the different assumption of values of D_i's, the details of the calculations are quite different.

2.2 THE RATE OF DISK INTERACTION

We start with the following two–dimensional diffusion equation:

$$\frac{\partial W}{\partial t} = D\nabla^2 W = D\left[\frac{\partial^2 W}{\partial x^2} + \frac{\partial^2 W}{\partial y^2}\right].$$

In polar form and by rotational symmetry, we have

$$\frac{\partial W}{\partial t} = D\left[\frac{\partial^2 W}{\partial r^2} + \frac{1}{r}\frac{\partial W}{\partial r}\right]$$

with boundary condition: $\omega(R,t) = 0 \quad \forall\, t > 0$

initial condition: $\omega(r,0) = \rho \quad |r| > R.$ (2.2.1)

In (2.2.1), let $y = W(r,t) - \rho$, then

$$\frac{\partial y}{\partial t} = D\left[\frac{\partial^2 y}{\partial r^2} + \frac{1}{r}\frac{\partial y}{\partial r}\right]$$

with boundary condition: $y(R,t) = -\rho \quad \forall t > 0$

initial condition: $y(r,0) = 0 \quad |r| > R\,.$ (2.2.2)

We take the Laplace Transformation of (2.2.2):

$$\mathscr{L}\left[\frac{\partial y}{\partial t}\right] = D\,\mathscr{L}\left[\frac{\partial^2 y}{\partial r^2} + \frac{1}{r}\frac{\partial y}{\partial r}\right]$$

or

$$s\ \hat{y} - y(r,0) = D\left[\frac{\partial^2}{\partial r^2}\ \hat{y} + \frac{1}{r}\ \frac{\partial}{\partial r}\ \hat{y}\right] \text{ where } \hat{y} = \mathscr{L}(y(r,t))$$

or

$$\frac{\partial^2 \hat{y}}{\partial r^2} + \frac{1}{r}\ \frac{\partial \hat{y}}{\partial r} - \frac{s}{D}\ \hat{y} = 0 \tag{2.2.3}$$

with boundary condition $\hat{y}(R,s) = \frac{-\rho}{s}$.

(2.2.2) is a modified Bessel Equation of order 0.

A solution is:

$$\hat{y}(r,s) = C_1(s)\ I_0\ \left[\sqrt{\frac{s}{D}}\ r\right] + C_2(s)\ K_0\ \left[\sqrt{\frac{s}{D}}\ r\right] \tag{2.2.4}$$

where $I_0(x)$ is a modified Bessel function of the first kind,

$K_0(x)$ is a modified Bessel function of the second kind.

But,

$$I_0(x) = \sum_{k=0}^{\infty} \frac{\left[\frac{1}{4}\ x^2\right]^k}{k!\ \Gamma(k+1)} ,$$

hence $I_0(x)$ is unbounded when x is large.

And also,

$$K_0(x) = -\left\{\ln\left[\frac{1}{2}\ x\right] + \gamma\right\}\ I_0(x) + \frac{\frac{1}{4}\ x^2}{(1!)^2}$$

$$+ \left[1 + \frac{1}{2}\right]\ \frac{\left[\frac{1}{4}\ x^2\right]^2}{(2!)^2} + \left[1 + \frac{1}{2} + \frac{1}{3}\right]\ \frac{\left[\frac{1}{4}\ x^2\right]^3}{(3!)!} + \ldots$$

where $$\gamma = \lim_{m\to\infty} \left[1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{m} - \ln\ m\right]$$

$$= .57721\ 56649\ \ldots$$

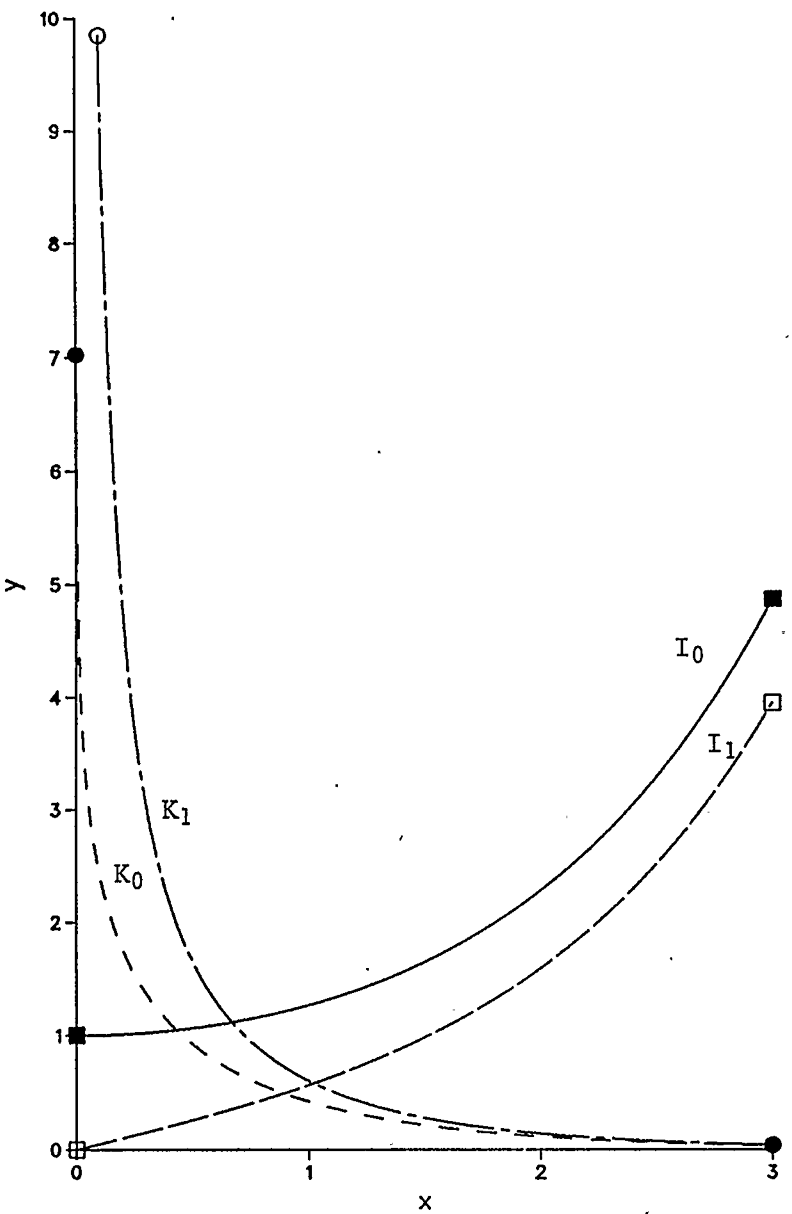


Figure 2.1. $I_0(x)$, $K_0(x)$, $I_1(x)$ and $K_1(x)$

hence $K_0(x)$ is bounded for all x.

The graph for $I_0(x)$, $K_0(x)$, $I_1(x)$ and $K_1(x)$ is shown in Figure 2.1.

The solution $\hat{y}(r,s)$ is bounded for all r, hence $C_1(s) = 0$, and from the boundary condition, we have

$$\frac{-\rho}{s} = C_2(s)\, K_0\left[\sqrt{\frac{s}{D}}\, R\right]$$

therefore

$$\hat{y}(r,s) = \frac{-\rho}{s}\, \frac{K_0\left[\sqrt{\frac{s}{D}}\, r\right]}{K_0\left[\sqrt{\frac{s}{D}}\, R\right]} . \tag{2.2.5}$$

Following the arguments of Smoluchowski, a circular disk of radius b is being fixed at the origin. At time t = 0, we assume all the circular disks have the same radius b, and are randomly scattered. When a circular disk touches the stationary disk they adhere, forming a double disk.

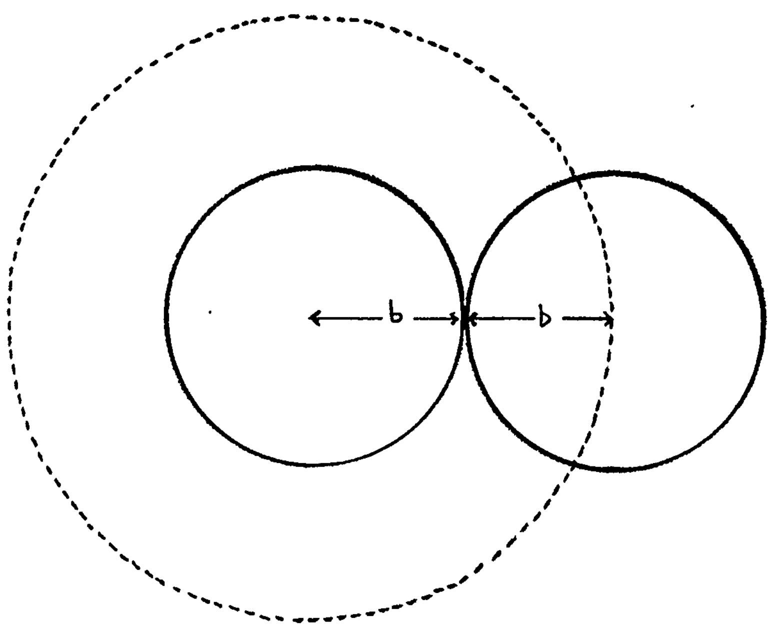


Figure 2.2

Since the primary disks adhere on contact, the rate of rouleaux formation equals the rate at which the centres diffuse across the dashed line. The latter corresponds to a circle of radius 2b inscribed around one of the disks which, for the present, is assumed to be stationary. In other words, we can assume a single circular disk of radius R = 2b at the origin and the other disks are redefined as points diffusing in the medium. When a disk, represented by a point touches at $|R| = 2b$, then we can regard it has merged with the central disk. The rate $\xi(R,t)$ at which disks merge with the central disk is:

$$\xi(R,t) = 2\pi RD \left.\frac{\partial \omega}{\partial r}\right|_{r=R}$$

or

$$\hat{\xi}(R,s) = 2\pi RD \left.\frac{\partial \hat{\omega}}{\partial r}\right|_{r=R}.$$

From (2.2.5), we have

$$\hat{\xi}(R,s) = 2\pi RD \frac{\partial}{\partial r}\left.\left[-\frac{\rho}{s}\frac{K_0\left[\sqrt{\frac{s}{D}}\, r\right]}{K_0\left[\sqrt{\frac{s}{D}}\, R\right]}\right]\right|_{r=R}$$

$$= -\, 2\pi RD \frac{\rho}{s\, K_0\left[\sqrt{\frac{s}{D}}\, R\right]} \frac{\partial}{\partial r} K_0 \left.\left[\sqrt{\frac{s}{D}}\, r\right]\right|_{r=R}. \qquad (2.2.6)$$

But

$$K_{\nu-1}(z) + K_{\nu+1}(z) = -\, 2\, K_\nu'(z)$$

and also

$$K_\nu(z) = K_{-\nu}(z)$$

hence

$$K_1(z) = -K_0'(z).$$

Therefore in (2.2.6), we have

$$\hat{\xi}(R,s) = \frac{2\pi RD\ \rho}{s}\sqrt{\frac{s}{D}}\ \frac{K_1\left[\sqrt{\frac{s}{D}}\ R\right]}{K_0\left[\sqrt{\frac{s}{D}}\ R\right]}$$

$$= 2\pi R\ \rho\sqrt{\frac{D}{s}}\ \frac{K_1\left[\sqrt{\frac{s}{D}}\ R\right]}{K_0\left[\sqrt{\frac{s}{D}}\ R\right]}\ . \qquad (2.2.7)$$

From Jaeger (1943), the inverse Laplace transform of (2.2.7) yields:

$$\xi(R,t) = \frac{8D}{\pi}\ \rho\ I\left[0,\ 1;\ \frac{Dt}{R^2}\right] \qquad (2.2.8)$$

where

$$I(0,1;\ x) = \int_0^\infty \frac{e^{-xu^2}}{J_0^2(u) + Y_0^2(u)}\ \frac{du}{u}\ ,$$

J_0: Bessel function of the first kind of order 0

and Y_0: Bessel function of the second kind of order 0.

A table of I(0,1,x) is given in Jaeger (1943).

If we remove the restriction that the 'target' disk is stationary, the effect is to replace the diffusion coefficient of the single moving disk with the relative diffusion coefficient of the two, which is simply 2D when the disks are the same size. Furthermore, instead of looking at a single disk, we may regard any one of the disks initially present as the 'reference' disk.

Therefore the rate r_{ij} at which disks of group size i with radius R_i combine with disks of group size j with radius R_j as a function of time t is:

$$r_{ij}(t) = \frac{8\ D_{ij}\ \nu_i \nu_j}{\pi}\ I\left[0,1;\ \frac{D_{ij}\ t}{R_{ij}^2}\right] \tag{2.2.9}$$

where

ν_i: average number of groups of size i per unit area.

R_{ij}: effective distance for formation of i+j – fold–disk group from groups of size i and j.

D_{ij}: effective diffusion constant for groups of size i and size j moving independently.

When a group of size i of radius R_i touch with a group of size j of radius R_j, they form an i + j fold group, hence $R_{ij} = R_i + R_j$. By independence of movements of each disk group, hence we have $D_{ij} = D_i + D_j$ (see Appendix I)

Initially, at time t = 0, we have only single disks only. There are no multiple disks at time t = 0, namely $\nu_i(0) = 0$ for i > 1. From then onwards, they combine to form double, triple, ... disks. In practice we begin our observation at a time $t_0 > 0$, at which time multiple groups may already exist. We will estimate the value of t_0 from experimental data.

The rate of change of various disk groups can be written as:

$$\frac{d\ \nu_1}{dt} = -\ \nu_1 \sum_j D_{1j}\ \nu_j\ f_{1j}(t) \tag{2.2.10}$$

and for $k \geq 2$, we have

$$\frac{d\,\nu_k}{dt} = \frac{1}{2} \sum_{i+j=k} \nu_i \nu_j \; f_{ij}(t) - \nu_k \sum_{j} D_{kj} \; \nu_j \; f_{kj}(t) \tag{2.2.11}$$

where

$$f_{ij} = \frac{8}{\pi} \, I\left[0,1; \; \frac{D_{ij}\,t}{R_{ij}^2}\right].$$

In equation (2.2.11), the first summation on the right hand side represents the increase in ν_k due to the formation of k–fold disk groups by coalescing of an i–fold and j–fold disk groups (i+j = k), the factor of $\frac{1}{2}$ must be included to account for duplication of indices in i+j = k. The second summation represents the decrease in ν_k due to the formation of (k+j)–fold disks in which one of the interacting disks is k–fold.

Furthermore, by adding (2.2.10) and (2.2.11) we have:

$$\frac{d}{dt} N_t = \frac{1}{2} \sum_{k=2} \sum_{i+j=k} \nu_i \nu_j \; D_{ij} \; f_{ij}(t) - \sum_{k=2} \nu_k \sum_{j} D_{kj} \; \nu_j \; f_{kj}(t)$$

$$- \nu_1 \sum_{j} D_{1j} \; \nu_j \; f_{1j}(t)$$

$$= \frac{1}{2} \sum_{i=1} \sum_{j=1} \nu_i \nu_j \; D_{ij} \; f_{ij}(t) - \sum_{k=1} \sum_{j=1} D_{kj} \; \nu_k \nu_j \; f_{kj}(t)$$

$$= -\frac{1}{2} \sum_{i=1} \sum_{j=1} \nu_i \nu_j \; D_{ij} \; f_{ij}(t) \tag{2.2.12}$$

where $N_t = \sum_{i=1} \nu_i$ which is the total number of disk groups at time t per unit area

In Chandrasekhar's paper, he assumed that

$$D_i = D_j \text{ and } R_i = R_j \text{ for all } i \text{ and } j.$$

It is not a very reasonable assumption since D_j is less than D_i for $i < j$ due to the increased mass. R_i is also less than R_j for $i < j$ due to the increased size. We will minimize these assumptions to find an upper bound for N_t^{-1} in Chapter III.

CHAPTER III

PLANAR BROWNIAN MOTION IN THE PRESENCE OF AN ATTRACTIVE FORCE

3.1 INTRODUCTION

In Chapter II, we solved the diffusion equation:

$$\frac{\partial W}{\partial t} = D\nabla^2 W$$

with boundary condition $W(R,t) = 0 \qquad \forall\ t > 0$

initial condition $W(r,0) = \rho \qquad \forall\ |r| > R$

and the rate $\xi(R,t)$ at which disk merge with the central disk was derived (eqn. 2.2.9). The rate r_{ij} at which disk of group size i with radius R_i combine with disks of group size j with radius R_j was also derived (eqn. 2.2.10). Furthermore, the rate of change of the number of cell groups $\frac{d}{dt} N_t$ was also found (eqn. 2.2.13).

In this chapter, we will derive an upper bound on N_t^{-1} and an example will be shown.

3.2 AN UPPER BOUND ON N_t^{-1}

If a force of attraction exists between the disk groups, the rate of formation of a rouleau is greater than that of free Brownian Movement. Hence N_t decreases more rapidly than in the free Brownian motion case. Suppose that the largest disk group of size m is observed in our observation and, for the sake of simplicity, assume m is even; if m is odd, the following argument will hold with m replaced by m+1. Since an increase in disk size reduces the velocity of its Brownian movements, the relative translational diffusion coefficient

$$D_{kq} = D_k + D_q \text{ attains its minimum when } k+q = m$$

i.e. $$D_{ij} \geqq D_{kq} \qquad \forall_{i,j} \quad \text{when} \quad k+q = m$$

equality holds when i+j = m. In particular, taking $k = \frac{m}{2}$, $q = \frac{m}{2}$, then we have $D_{ij} \geqq D_{\frac{m}{2}\frac{m}{2}} = 2\, D_{\frac{m}{2}}$, $\forall_{i,j}$.

By the Stokes–Einstein relation (Marshall, 1978)

$$\begin{aligned} D_i R_i &= \frac{kT}{6\pi\eta} \\ &= \text{constant for all groups} \end{aligned}$$

Moreover, $$D_{ij}\, R_{ij} = D_{\frac{m}{2}\frac{m}{2}}\, R_{\frac{m}{2}\frac{m}{2}} \qquad \forall_{i,j}$$

or

$$\frac{D_{ij}}{D_{\frac{m}{2}\frac{m}{2}}} R_{ij} = R_{\frac{m}{2}\frac{m}{2}} = 2\, R_{\frac{m}{2}}$$

but $$\frac{D_{ij}}{D_{\frac{m}{2}\frac{m}{2}}} \geqq 1, \text{ hence}$$

$$R_{ij} \leqq 2\, R_{\frac{m}{2}} \; .$$

Therefore, we can conclude that for any time t,

$$\frac{D_{ij}\,t}{R_{ij}^2} \geq \frac{D_{\frac{m}{2}}\ t}{2\ R_{\frac{m}{2}}^2}. \tag{3.2.1}$$

But I(0,1; x) is a decreasing function of x and hence

$$I\left[0,1;\ \frac{D_{ij}\,t}{R_{ij}^2}\right] \leq I\left[0,1;\ \frac{D_{\frac{m}{2}}\ t}{2\ R_{\frac{m}{2}}^2}\right]. \tag{3.2.2}$$

Therefore we have an upper bound for $f_{ij}(t)$, namely

$$f_{ij}(t) = \frac{8}{\pi}\, I\left[0,1;\ \frac{D_{ij}\,t}{R_{ij}^2}\right] \leq r(t) = \frac{8}{\pi}\, I\left[0,1;\ \frac{D_{\frac{m}{2}}\ t}{2\ R_{\frac{m}{2}}^2}\right]. \tag{3.2.3}$$

Let us assume $D_1 = D$, $D_2 = \alpha\, D$, $D_i = \alpha\, \beta\, D$, $i \geq 3$ where α, $\beta \in (0,1]$. This is a reasonable assumption since D_i decreases when i increases. We will use experimental results to estimate α and β. We can make further refinements for D_4, D_5 etc., but it was found that the results were not sensitive to variations in α and β. Hence further refinement is not necessary. For notational convenience, let:

$$y_1 = D\ \hat{\nu}_1,\ y_2 = D\ \hat{\nu}_2,\ y_3 = D\ \hat{N}_t,$$

where $\hat{\nu}_1$, $\hat{\nu}_2$, $\hat{N}_t$ are calculated values of ν_1, ν_2, N_t under the above assumptions. In order to obtain an upper bound on N_t^{-1}, we replace $f_{ij}(t)$ by r(t),

$$\frac{d\hat{\nu}_1}{dt} = -\hat{\nu}_1 (D_{11}\hat{\nu}_1 + D_{12}\hat{\nu}_2 + D_{13}\hat{\nu}_3 + \ldots.)\, r(t)$$

$$= -D\left[2\hat{\nu}_1^2 + (1+\alpha)\,\hat{\nu}_1\hat{\nu}_2 + (1+\alpha\beta)\,\hat{\nu}_1 \sum_{j=3} \nu_j\right] r(t)$$

$$= -D\left[2\hat{\nu}_1^2 + (1+\alpha)\,\hat{\nu}_1\hat{\nu}_2 + (1+\alpha\beta)\,\hat{\nu}_1 (\hat{N}_t - \hat{\nu}_1 - \hat{\nu}_2)\right] r(t).(3.2.4)$$

$$\frac{dy_1}{dt} = D\frac{d}{dt}\hat{\nu}_1 = -D^2\left[2\hat{\nu}_1^2 + (1+\alpha)\,\hat{\nu}_1\hat{\nu}_2 + (1+\alpha\beta)\,\hat{\nu}_1 (\hat{N}_t - \hat{\nu}_1 - \hat{\nu}_2)\right] r(t)$$

$$= -\left\{2\,y_1^2 + (1+\alpha)\,y_1y_2 + (1+\alpha\beta)\,y_1\,(y_3 - y_1 - y_2)\right\} r(t)$$

$$= -\left\{y_1^2\,(1-\alpha\beta) + (1-\beta)\,\alpha\,y_1y_2 + (1+\alpha\beta)\,y_1\,y_3\right\} r(t)\,. \qquad (3.2.5)$$

Similarly,

$$\frac{dy_3}{dt} = D\frac{d}{dt}\hat{N}_t = -\frac{D}{2}\sum_i \sum_j \hat{\nu}_i\hat{\nu}_j\,(D_i + D_j)\, r(t).$$

$$= -\frac{D}{2}\left[\hat{\nu}_1^2\,(D_1+D_1) + 2\,\hat{\nu}_1 \sum_{j=2} \hat{\nu}_j\,(D_1+D_j)\right.$$

$$\left. + \sum_{i\,,} \sum_{j\geq 2} \hat{\nu}_i\hat{\nu}_j\,(D_i + D_j)\right] r(t) \qquad (3.2.6)$$

$$= -\Big\{y_1^2 + (1+\alpha)\ y_1y_2 + y_1(1+\alpha\beta)(y_3-y_1-y_2) + \alpha\ y_2^2$$

$$+\ \alpha(1+\beta)(y_3-y_1-y_2)\ y_2 + \alpha\beta(y_3-y_1-y_2)^2\Big\}\ r(t)$$

$$= -\Big\{(1-\alpha\beta)\ \ y_1y_3 + (1-\beta)\ \alpha\ y_2y_3 + \alpha\beta\ y_3^2\Big\}\ r(t). \qquad (3.2.7)$$

Again,

$$\frac{dy_2}{dt} = D\ \frac{d}{dt}\ \hat{\nu}_2 = \frac{D}{2} \sum_{i+j=2} \hat{\nu}_i\hat{\nu}_j\ D_{ij}\ r(t) - \hat{\nu}_2 \sum_{j=1} \hat{\nu}_j\ D_{2j}\ r(t)$$

$$= \Big[y_1^2 - y_1y_2(1+\alpha) - 2\alpha\ y_2^2 - y_2(1+\beta)\ \alpha\{y_3 - y_1 - y_2\}\Big]\ r(t)$$

$$= \Big[y_1^2 - (1-\alpha\beta)\ y_1y_2 - \alpha(1-\beta)\ y_2^2 - \alpha(1+\beta)\ y_2y_3\Big]\ r(t). \qquad (3.2.8)$$

Dividing (3.2.4) by (3.2.8), we have

$$\frac{d\ y_1}{d\ y_2} = \frac{y_1^2\ (1-\alpha\beta) + (1-\beta)\ \alpha\ y_1y_2 + (1+\alpha\beta)\ y_1y_3}{-\ y_1^2 + (1-\alpha\beta)\ \ y_1y_2 + \alpha(1-\beta)\ y_2^2 + \ \alpha(1+\beta)\ y_2y_3}\ . \qquad (3.2.9)$$

Dividing (3.2.4) by (3.2.7), we have

$$\frac{d\ y_1}{d\ y_3} = \frac{y_1^2\ (1-\alpha\beta) + (1-\beta)\ \alpha\ y_1y_2 + (1+\alpha\beta)\ y_1y_3}{(1-\alpha\beta)\ \ y_1y_3 + (1-\beta)\ \ \alpha\, y_2y_3 + \alpha\ \ \beta\, y_3^2}\ . \qquad (3.2.10)$$

Let $u = \frac{y_1}{y_3}$, $v = \frac{y_2}{y_3}$, $\quad 0 \leq u, v \leq 1.$

Therefore

$$\frac{dy_1}{dy_3} = \frac{u^2\ y_3^2(1-\alpha\beta)+(1-\beta)\ \alpha\ u\ y_3\ v\ y_3+(1+\alpha\beta)\ u\ y_3^2}{(1-\alpha\beta)\ u\ y_3^2 + (1-\beta)\ \alpha\ v\ y_3^2 + \alpha\ \beta\ y_3^2}$$

$$= \frac{u^2(1-\alpha\beta) + (1-\beta)\ \alpha\ u\ v + (1+\alpha\beta)\ u}{(1-\alpha\beta)\ u + (1-\beta)\ \alpha\ v + \alpha\beta}$$

or
$$y_3\ \frac{du}{dy_3} = \frac{u}{(1-\alpha\beta)\ u + (1-\beta)\ \alpha\ v + \alpha\beta}\ . \tag{3.2.11}$$

Similarly

$$v + y_3\ \frac{dv}{dy_3} = \frac{-u^2 + u\ v(1-\alpha\beta) + v^2\ \alpha(1-\beta) + \alpha\,(1+\beta)\ v}{(1-\alpha\beta)\ u + (1-\beta)\ \alpha\ v + \alpha\beta}$$

or
$$y_3\ \frac{dv}{dy_3} = \frac{-\ u^2 + \alpha v}{(1-\alpha\beta)\ u + (1-\beta)\ \alpha\ v + \alpha\beta} \tag{3.2.12}$$

dividing (3.2.12) by (3.2.11) we have

$$\frac{dv}{du} = \frac{\alpha v}{u} - u \tag{3.2.13}$$

with initial condition $u(0) = 1$, $v(0) = 0$.

This linear differential equation has solution

$$v = cu^{\alpha} - \frac{u^2}{2-\alpha} \tag{3.2.14}$$

At time $t = t_0$, our initial observed time,

$$N_{t_0} = N_1,\ u(t_0) = u_1 = \frac{\nu_1(t_0)}{N_1}$$

$$v(t_0) = v_1 = \frac{\nu_2(t_0)}{N_1}$$

and therefore
$$C = \left[v_1 + \frac{u_1^2}{2-\alpha}\right] u_1^{-\alpha} . \tag{3.2.15}$$

Combining (3.2.15) and (3.2.11), we have

or
$$\left[\alpha\beta + (1-\alpha\beta)\ u + (1-\beta)\ \alpha(C\ u^\alpha - \frac{u^2}{2-\alpha})\right] \frac{du}{u} = \frac{dy_3}{y_3}$$

or
$$\ell n\ y_3 = \alpha\beta\ \ell n\ u + (1-\alpha\beta)\ u + (1-\beta)\ \alpha\left[C\ \frac{u^\alpha}{\alpha} - \frac{u^2}{2(2-\alpha)}\right] + C'$$

or
$$y_3 = K\ u^{\alpha\beta} \exp\left\{(1-\alpha\beta)\ u + \frac{1-\beta}{2(2-\alpha)}\ (2C\ (2-\alpha)\ u^\alpha - \alpha\ u^2)\right\} . \tag{3.2.16}$$

At, $t = t_0$

$$y_3 = K\ u_1^{\alpha\beta} \exp\left\{(1-\alpha\beta)\ u_1 + \frac{1-\beta}{2(2-\alpha)}\ (2C\ (2-\alpha)\ u_1^\alpha - \alpha\ u_1^2)\right\}$$

or $$K = D\ N_{t_0}\ u_1^{-\alpha\beta} \exp\left\{-\left[(1-\alpha\beta)\ u_1 + \frac{(1-\beta)}{2}\ (2v_1 + u_1^2)\right]\right\}.$$

Recall $y_2 = vy_3$, we have

$$\frac{dy_2}{dt} = v\ \frac{dy_3}{dt} + y_3\ \frac{dv}{dt}$$

and therefore

$$y_3\ \frac{dv}{dt} = -\left[-\ y_1^2 + (1-\alpha\beta)\ y_1y_2 + \alpha(1-\beta)\ y_2^2 + \alpha(1+\beta)\ y_2y_3\right]\ r(t)$$
$$+\ v\left[(1-\alpha\beta)\ y_1y_3 + \alpha(1-\beta)\ y_2y_3 + \alpha\beta\ y_3^2\right]\ r(t)$$

or $$\frac{dv}{dt} = \{u\ y_1 - \alpha\ y_2\}\ r(t).$$

But from (3.2.13)

$$\frac{du}{dv} = \frac{\frac{du}{dt}}{\frac{dv}{dt}} = \frac{u}{\alpha v - u^2}$$

therefore

$$\frac{du}{dt} = \frac{u}{\alpha v - u^2}\ \frac{dv}{dt}$$

$$= \frac{u}{\alpha v - u^2}\ \{u\ y_1 - \alpha\ y_2\}\ r(t)$$

$$= \frac{u}{\alpha v - u^2}\ \{u^2\ y_3 - \alpha\ v\ \dot{y}_3\}\ r(t)$$

$$= \frac{u}{\alpha v - u^2}\ \{u^2 - \alpha\ v\}\ y_3\ r(t)$$

$$= -\ u\ y_3\ r(t)$$

i.e. $\frac{du}{dt} = - u \; y_3 \; r(t)$

$$\text{therefore} \int_{u_1}^{u(t)} \frac{du}{uy_3} = - \int_{t_0}^{t} r(t) \; dt.$$

$$= - \frac{8}{\pi} \int_{t_0}^{t} I\left[0,1; \frac{D_{\frac{m}{2}} t}{2R^2_{\frac{m}{2}}}\right] dt$$

$$= - \frac{16 R^2_{\frac{m}{2}}}{\pi D_{\frac{m}{2}}} \int_{y_0}^{y} I(0,1; \; x) \; dx \qquad (3.2.17)$$

where $\quad y_0 = \frac{D_{\frac{m}{2}} t_0}{2R^2_{\frac{m}{2}}}$ and $y = \frac{D_{\frac{m}{2}} t}{2R^2_{\frac{m}{2}}}$.

Next, we want to find an estimate of t_0:

$$\frac{dy_3}{dt} = D \frac{d}{dt} \hat{N}_t = - \{(1-\alpha\beta) \; y_1 y_3 + (1-\beta) \; \alpha y_2 y_3 + \alpha\beta \; y_3^2\} \; r(t)$$

$$= - y_3^2 \; \{(1-\alpha\beta) \; u + (1-\beta) \; \alpha v + \alpha\beta\} \; r(t),$$

so that $\quad r(t) = \frac{-1}{D \; \hat{N}_t^2} \left[\frac{d}{dt} \hat{N}_t\right] \frac{1}{\alpha\beta + (1-\alpha\beta)u + \alpha(1-\beta)v}$,

and so
$$r(t_0) = \frac{1}{D}\frac{d}{dt}\frac{1}{\hat{N}_t}\bigg|_{t=t_0}\left[\frac{1}{\alpha\beta+(1-\alpha\beta)u_1+\alpha(1-\beta)v_1}\right]. \qquad (3.2.18)$$

Empirically finding $\frac{d}{dt}\frac{1}{\hat{N}_t}\bigg|_{t=t_0}$ we can find $r(t_0)$. From Jaeger's table, we can find t_0 from the calculated value of $r(t_0)$ in (3.2.18). For known values of t_0, u_1, v_1, we can perform the numerical integration in (3.2.17). Hence, from (3.2.17) we can calculate y_3 and $\hat{N}_t^{-1} = \frac{D}{y_3}$ can be calculated. Finally, we use an example to complete our present chapter.

EXAMPLE

Experiments were conducted in which a cell suspension in plasma was transferred to a haemacytometer chamber and allowed to settle. By using time–lapse cine microphotography of erythrocytes, it was possible to count the total number of red cells and rouleaux in a fixed region as a function of time t. A complete description of the experimental procedure is in Rowlands et al (1982).

Experimental evidence suggests that the diffusion coefficient of a single cell is $D = 1.596 \times 10^{-14}$ m^2s^{-1} while for double and triple cells it is 0.86D and 0.73D respectively: i.e. $\alpha = 0.86$, $\beta = 0.8488$. We tried several values of α, β but the results were found to be insensitive to variations of α and β.

Observation was started at time t_0, initial counting gave $u_1 = 0.9$ and $v_1 = 0.1$. The maximum group size that we observed in time interval $[t_0, t + t_0]$ was 6, hence m = 6. Also the radius of a single cell is taken as $R = 4.3 \times 10^{-6}$ m. The data used in our calculation are in Table 3.1.

For PH = 7.4 or live cells, by cubic spline approximation (use ICSCCU in IMSL), we find:

$$\frac{d}{dt}\frac{1}{N(t)}\bigg|_{t=t_0} = 51.57 \times 10^{-14}$$

which yields $$r(t_0) = 32.7707.$$

Therefore $$I(0,1;\, x) = \frac{\pi}{8}\, r(t_0) = 12.869.$$

Using $D_3R_3 = D_1R_1$, we have $R_3 = \frac{R_1}{0.73} = 5.89 \times 10^{-6}$m.

Jaeger's table (1943), then gives

$$\frac{D_3 t_0}{2R_3^2} = 0.02$$

from which $$t_0 = 119.9 \text{ sec.}$$

Since t_0 is found and $u_1 = 0.9$, hence in (3.2.18), for any given value of t, we can find out the value of u(t), and hence N_t^{-1} can be calculated. The graph of N_t^{-1} versus t is plotted in Figure 3.1. The smooth curve is the theoretical curve of the upper bound of N_t^{-1}. The points in the graph are the experimental data. In Figure 3.1, the data points lie above the theoretical curve, hence there is an evidence that a force of attraction exists among the cell groups other than the Brownian Motion.

For PH = 6.3, or dead cells, as for PH = 7.4, we find:

$$\frac{d}{dt}\left.\frac{1}{N(t)}\right|_{t=t_0} = 13.679 \times 10^{-14}$$

$$r(t_0) = 8.69245$$

$$I\left[0,1;\ \frac{D_3 t_0}{2R_3^2}\right] = 3.4135.$$

$$\frac{D_3 t_0}{2R_3^2} = 0.35$$

$$t_0 = 2084.4 \text{ sec.}$$

In Figure 3.2, the data points lie below the theoretical curve as would be expected for Brownian Motion only.

TABLE 3.1a* (PH = 7.4)

Observed time (minute)	Number of cell groups observed in an area of 1.2×10^{-7} m^2
0	188
5	164
10	154
15	131
20	129
30	118
40	110
50	106
60	96
70	86
75	86

TABLE 3.1b* (PH = 6.3)

Observed time (minute)	Number of cell groups observed in an area of 1.2×10^{-7} m^2
0	227
5	213
10	204
15	199
20	192
30	186
40	185
50	177
60	179
70	174
80	169
90	166
100	163
110	164
120	161

*Source : S. Rowlands and L.S. Sewchand.

Comment : The number of cell groups increases twice. This is due to the fact that we are observing the central region of our viewing area and cells can freely enter and leave our viewing area.

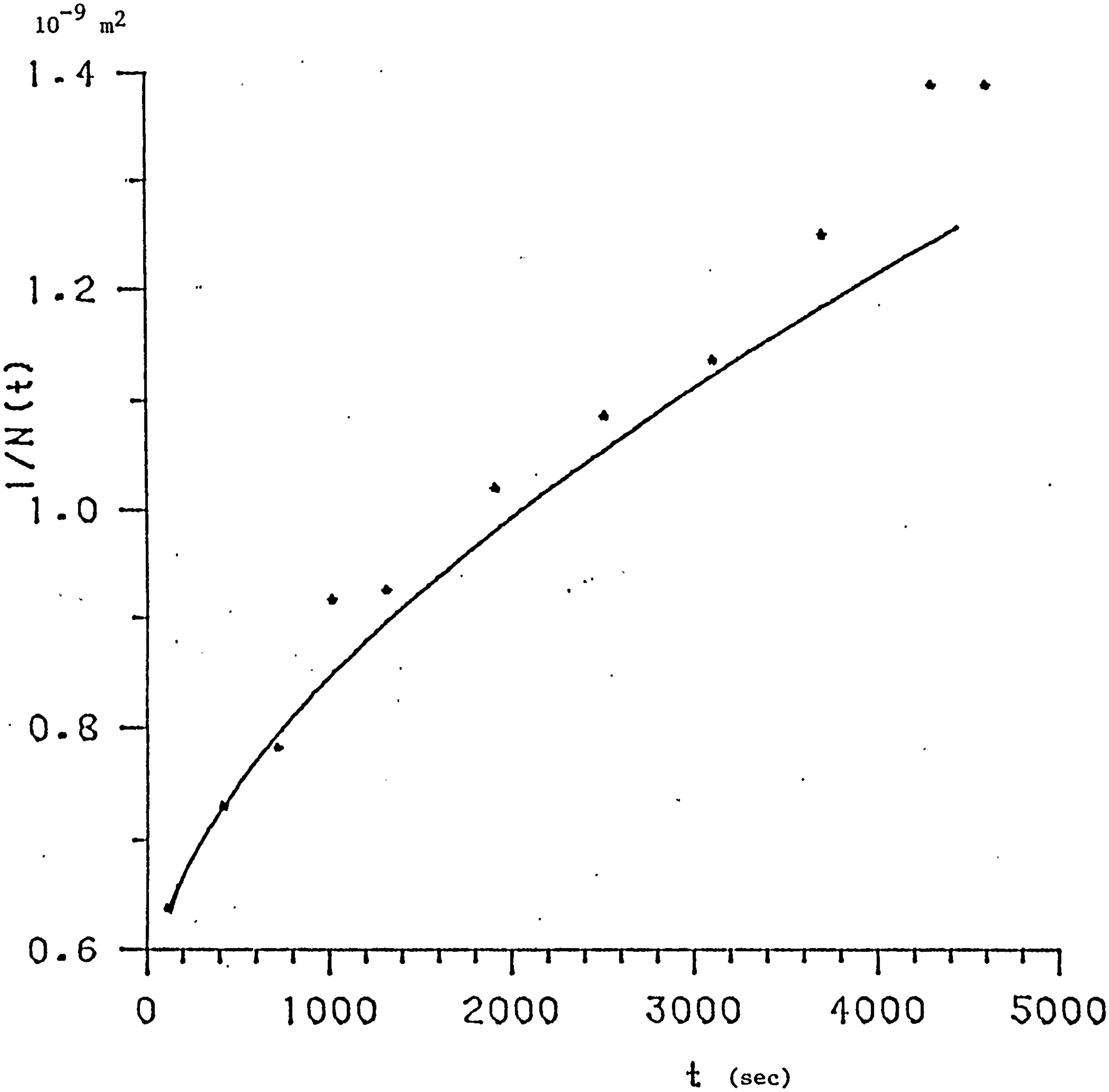


FIGURE 3.1. Brownian motion of erythrocytes at pH 7.4

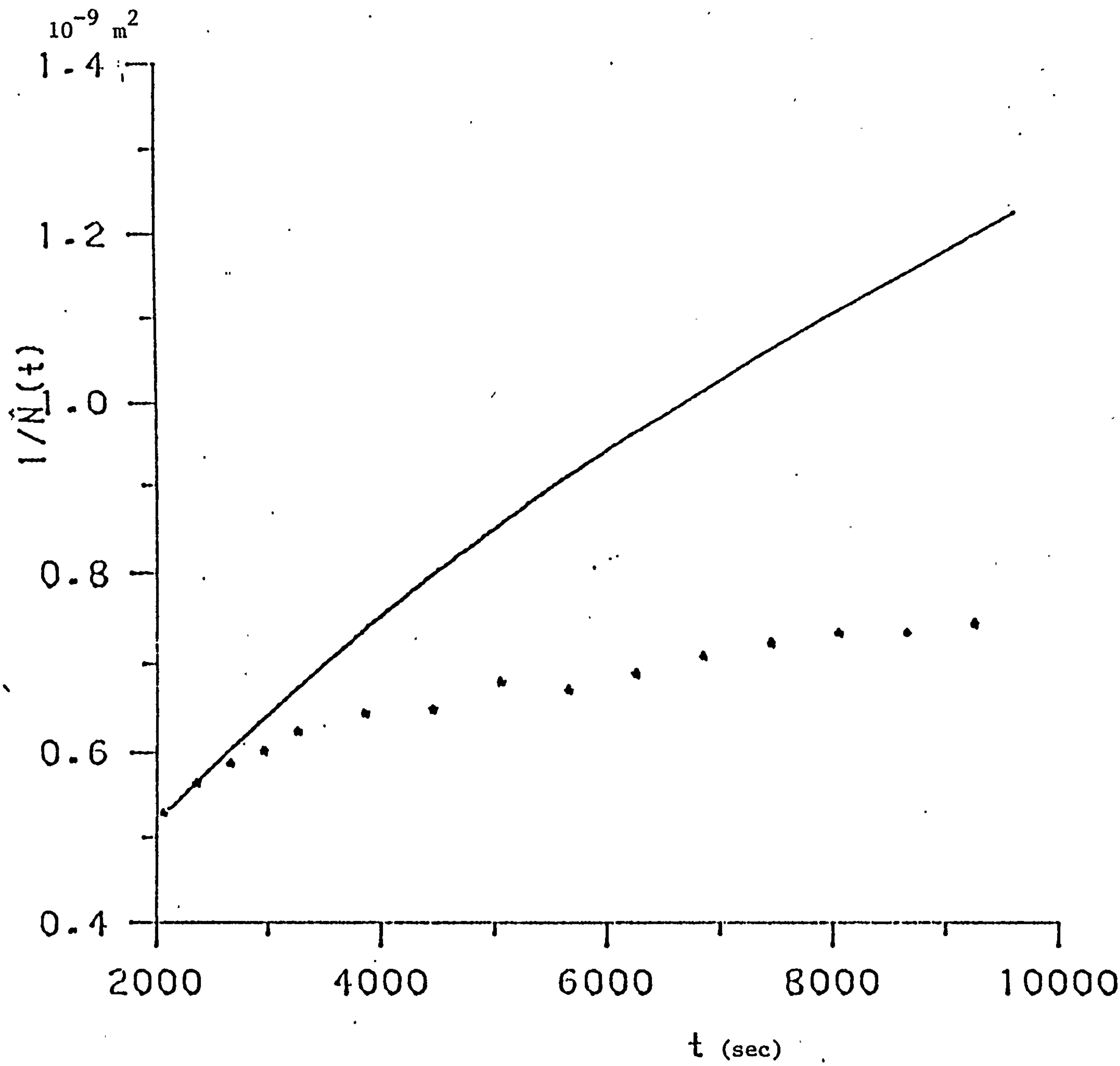


FIGURE 3.2. Brownian motion of erythrocytes at pH 6.3.

3.3 DISCUSSION OF THE MODEL

In general, the particles of any particular class will not be spheres. So, one must incorporate some factor relating the Stokes radius of each aggregate particle to that of the fundamental particle. In turn, the Stokes radius of the fundamental particle must be related to a characteristic geometric radius. The mathematical model that has been developed is under the assumption that the Stokes radii of all classes are equal to their physical radii. This has been confirmed reasonably well for erythrocytes (Groom & Anderson, 1972; Skalak et al, 1981).

Points lying below the upper bound of N_t^{-1} indicates that cells are executing free Brownian motion. This is a crucial statement, one may derive a lower bound of N_t^{-1}, then cells with all data points lying within the lower bound and upper bound of N_t^{-1}, one can claim that such cells are executing free Brownian motion.

Cells which lie outside these bounds would give us an indication that the cells have some type of force acting in conjunction with Brownian motion.

CHAPTER IV

HITTING PROBABILITIES FOR n–DIMENSIONAL BROWNIAN MOTION

4.1 INTRODUCTION:

Consider an n–sphere of radius b held stationary at the origin of our system of co–ordinates and in a medium of infinite extent in which a number of Brownian particles of zero radius are scattered at time t = 0. Our familiar diffusion can be expressed as:

$$\frac{\partial w}{\partial t} = D\nabla^2 w = D\left[\frac{\partial^2 w}{\partial x_1^2} + \frac{\partial^2 w}{\partial x_2^2} + \cdots + \frac{\partial^2 w}{\partial x_n^2}\right]$$

where w is the concentration of the particles in the system.

By radial symmetry and n–sphere polar co–ordinates, we have

$$\frac{\partial w}{\partial t} = D\left[\frac{\partial^2 w}{\partial r^2} + \frac{n-1}{r}\frac{\partial w}{\partial r}\right]$$

with boundary condition $w(b,t) = 0 \qquad \forall\ t > 0$

initial condition $w(r,0) = \rho \qquad \forall\ |r| > b.$ (4.1.1)

Using the same argument as in Chapter 2.2,

let $y = w(r,t) - \rho$; then

$$\frac{\partial y}{\partial t} = D\left[\frac{\partial^2 y}{\partial r^2} + \frac{n-1}{r}\frac{\partial y}{\partial r}\right]$$

with boundary condition $y(b,t) = -\rho \qquad \forall\ t > 0$

and initial condition $y(r,0) = 0 \qquad |r| > b.$ (4.1.2)

The Laplace Transform of (4.1.2), is then

$$D\left[\frac{\partial^2 \hat{y}}{\partial r^2} + \frac{n-1}{r}\frac{\partial \hat{y}}{\partial r}\right] = s\ \hat{y} - y(r,0)$$

where $\hat{y} = \mathscr{L}(y(r,t))$

or

$$\frac{\partial^2 \hat{y}}{\partial r^2} + \frac{n-1}{r}\frac{\partial \hat{y}}{\partial r} - \frac{s}{D}\hat{y} = 0$$

with boundary condition $\hat{y}(b,s) = \frac{-\rho}{s}$. (4.1.3)

By Gradshteyn and Ryzik (1965) page 971 and regularity of $K_n(x)$ when $x \to \infty$, the solution of (4.1.3) is

$$\hat{y}(r,s) = \frac{-\rho}{s}\left[\frac{b}{r}\right]^{\frac{n}{2}-1} \frac{K_{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\ r\right]}{K_{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\ b\right]} . \tag{4.1.4}$$

The rate $\xi(b,t)$ at which particles merge with the central n–sphere with radius b is:

$$\xi(R,t) = \text{surface area of n–sphere} \cdot D \cdot \frac{\partial y}{\partial r}(r,t)\Big|_{r=b}$$

or

$$\xi(R,s) = nC_n\ r^{n-1} \cdot D \cdot \frac{\partial \hat{y}}{\partial r}(r,s)\Big|_{r=b}$$

where $C_n = \dfrac{2\pi^{n/2}}{n\Gamma\left[\frac{n}{2}\right]}$ is the volume of the unit n–sphere. (4.1.5)

But
$$\frac{\partial\hat{y}}{\partial r}(r,s) = \frac{-\rho}{s}\,\frac{b^{\frac{n}{2}-1}}{K_{\frac{n}{2}-1}\left(\sqrt{\frac{s}{D}}\,b\right)}\left\{r^{-n/2}\left(1-\frac{n}{2}\right)K_{\frac{n}{2}-1}\left(\sqrt{\frac{s}{D}}\,r\right)\right.$$
$$\left. + \sqrt{\frac{s}{D}}\,r^{1-\frac{n}{2}}\,K'_{\frac{n}{2}-1}\left(\sqrt{\frac{s}{D}}\,r\right)\right\}. \qquad (4.1.6)$$

Using the identity (Watson, page 79):

$$zK'_n(z) - nK_n(z) = -\,zK_{n+1}(z)$$

(4.1.6) becomes

$$\frac{\partial\hat{y}}{\partial r}(r,s) = \frac{\rho}{s}\,\frac{b^{\frac{n}{2}-1}}{K_{\frac{n}{2}-1}\left(\sqrt{\frac{s}{D}}\,b\right)}\,r^{-n/2}\left\{\sqrt{\frac{s}{D}}\;r\,K_{\frac{n}{2}}\left(\sqrt{\frac{s}{D}}\,r\right)\right\}$$

and therefore

$$\left.\frac{\partial\hat{y}}{\partial r}(r,s)\right|_{r=b} = \frac{\rho}{s}\sqrt{\frac{s}{D}}\,\frac{K_{\frac{n}{2}}\left(\sqrt{\frac{s}{D}}\,b\right)}{K_{\frac{n}{2}-1}\left(\sqrt{\frac{s}{D}}\,b\right)}. \qquad (4.1.7)$$

Putting (4.1.7) into (4.1.5) we have

$$\hat{\xi}(b,s) = nC_n\,b^{n-1}\,D\,\frac{\rho}{s}\sqrt{\frac{s}{D}}\,\frac{K_{\frac{n}{2}}\left(\sqrt{\frac{s}{D}}\,b\right)}{K_{\frac{n}{2}-1}\left(\sqrt{\frac{s}{D}}\,b\right)}. \qquad (4.1.8)$$

4.2 TWO DIMENSIONAL HITTING PROBABILITIES

Imagine a Brownian particle beginning at distance R from the centre of a stationary circle of radius b and define R(t) as its distance at time t. We want the probability of the Brownian particle hitting the stationary circle after a duration of time t.

We define:

$$F(b,t;\ R) = P\{R(t) \le b \mid R(0) = R\}$$

$$\tau = \min[t\colon\ R(t) \le b \mid R(0) = R]$$

$$G(b,t;\ R) = \begin{cases} P\{\tau \le t\} & R > b \\ 1 & R \le b \end{cases}$$

$$\hat{F}(b,s;\ R) = \int_0^{\infty} e^{-st}\ F(b,t;\ R)\ dt$$

$$\hat{G}(b,s;\ R) = \int_0^{\infty} e^{-st}\ G(b,t;\ R)\ dt\ .$$

From the above definition, F(b,t; R) satisfies the backward diffusion equation, namely,

$$\frac{\partial F}{\partial t} = D\left[\frac{\partial^2 F}{\partial R^2} + \frac{1}{R}\frac{\partial F}{\partial R}\right]\ . \qquad (4.2.1)$$

See Karlin & Taylor (1981) pages 214–216.

Taking Laplace Transform on (4.2.1), we have

$$s\ \hat{F} = D\left[\frac{\partial^2 \hat{F}}{\partial R^2} + \frac{1}{R}\frac{\partial \hat{F}}{\partial R}\right]$$

or equivalently,

$$\frac{\partial^2 \hat{F}}{\partial R^2} + \frac{1}{R}\frac{\partial \hat{F}}{\partial R} - \frac{s}{D}\hat{F} = 0. \qquad (4.2.2)$$

The general solution of (4.2.2) is

$$\hat{F}(b,s;\ R) = A\ I_0\left[\sqrt{\frac{s}{D}}\ R\right] + B\ K_0\left[\sqrt{\frac{s}{D}}\ R\right]$$

where A, B may depend on s and on b.

As $R \to \infty$, only K_0 is bounded, therefore $A = 0$ and

$$\hat{F}(b,s;\ R) = B(s,b)\ K_0\left[\sqrt{\frac{s}{D}}\ R\right].$$

By continuity of the sample functions and the Markovian nature of the process $R(t)$, we have, for $b \leq R$,

$$F(b,t;\ R) = \int_0^t F(b,t-x;\ b) \cdot g(b,x;\ R)\ dx$$

$$= \int_0^t F(b,t-x;\ b)\ d_x\ G(b,x;\ R). \qquad (4.2.3)$$

Since

$$\mathscr{L}\left[\int_0^t F(t-u)\ g(u)\ du\right] = \hat{F}(s)\ \hat{g}(s)$$

$$= \hat{F}(s)\ .\mathscr{L}(\hat{G}'(u))$$

and

$$\mathscr{L}(G'(b,s;\ R)) = s\ \hat{G}(b,s;\ R) - G(b,0;\ R)$$

$$= s\ \hat{G}(b,s;\ R),$$

therefore by taking the Laplace Transform of (4.2.3), we have:

$$\hat{F}(b,s;\ R) = \hat{F}(b,s;\ b) \cdot s \cdot \hat{G}(b,s;\ R)$$

or

$$\hat{G}(b,s;\ R) = \frac{1}{s}\,\frac{\hat{F}(b,s;\ R)}{\hat{F}(b,s;\ b)}$$

$$= \frac{1}{s}\,\frac{K_0\left[\sqrt{\frac{s}{D}}\,R\right]}{K_0\left[\sqrt{\frac{s}{D}}\,b\right]}\,. \qquad (4.2.4)$$

Let Y_R denote the first hitting time of a Brownian particle p_1 with initial distance R from the centre of the circle, then

$$E(e^{-sY_R}) = \int_0^\infty e^{-st}\,dP\{Y_R \le t\}$$

$$= e^{-st}\,P\{Y_R \le t\}\Big|_{t=0}^{t=\infty} + s\int_0^\infty P\{Y_R \le t\}\,e^{-st}\,dt$$

$$= s\,\hat{G}(b,s;\ R) = \frac{K_0\left[\sqrt{\frac{s}{D}}\,R\right]}{K_0\left[\sqrt{\frac{s}{D}}\,b\right]}\,. \qquad (4.2.5)$$

The particle p_1 under consideration was randomly placed within the region $b < r \leqq a$, such that the density function of it's distance to the origin is:

$$f(r) = \begin{cases} \frac{2r}{a^2-b^2} & b < r \leqq a \\ 0 & \text{otherwise} \end{cases}\,. \qquad (4.2.6)$$

Define τ to be the time for p_1 to hit the inner circle, then

$$P(\tau \leq t) = \int_b^a P(Y_r \leq t) \frac{2r}{a^2-b^2} dr$$

$$= \frac{2}{a^2-b^2} \int_b^a r\, P(Y_r \leq t)\, dr \; . \tag{4.2.7}$$

If N points are independently and randomly placed in the region $b < r \leq a$, then (4.2.7) may be written as:

$$P(\tau \leq t) = \frac{2\pi\rho}{N} \int_b^a P(Y_r \leq t)\, rdr \tag{4.2.8}$$

where $\rho = \frac{N}{\pi(a^2-b^2)}$ i.e. ρ is the density of particles.

If T_N is the time until the first of the N particles collides with the central circle, then

$$P(T_N > t) = [P(\tau > t)]^N.$$

Let N and a approach ∞ so that the density ρ remains constant. If T is the time until first absorption for points with initial density ρ, then

$$P(T > t) = \lim_{\substack{N\to\infty \\ a\to\infty}} P(T_N > t)$$

$$= \lim_{\substack{N\to\infty \\ a\to\infty}} [1 - P(\tau \leq t)]^N$$

$$= \lim_{\substack{N\to\infty \\ a\to\infty}} \left[1 - \frac{2\pi\rho}{N} \int_b^a P(Y_r \leq t)\, rdr\right]^N$$

$$= e^{-2\pi\rho \int_b^\infty P(Y_r \leq t)\, rdr} \; . \tag{4.2.9}$$

But $\mathscr{L}\left[\int_b^\infty P(Y_r \le t)\ rdr\right] = \int_{t=0}^\infty \int_{r=b}^\infty e^{-st}\ P(Y_r \le t)\ rdr\ dt$

$$= \frac{1}{s} \int_b^\infty r\ \frac{K_0\left[\sqrt{\frac{s}{D}}\ r\right]}{K_0\left[\sqrt{\frac{s}{D}}\ b\right]}\ dr$$

$$= \frac{1}{s}\ \frac{b}{\sqrt{\frac{s}{D}}}\ \frac{K_1\left[\sqrt{\frac{s}{D}}\ b\right]}{K_0\left[\sqrt{\frac{s}{D}}\ b\right]}\ . \tag{4.2.10}$$

From equation (4.1.8) i.e. $\hat{\xi}(b,s) = 2\pi\rho\ \frac{b}{\sqrt{\frac{s}{D}}}\ \frac{K_1\left[\sqrt{\frac{s}{D}}\ b\right]}{K_0\left[\sqrt{\frac{s}{D}}\ b\right]}$ we have

$$\mathscr{L}\left[\int_b^\infty P(Y_r \le t)\ rdr\right] = \frac{\hat{\xi}\,(b,s)}{s\ 2\pi\rho}$$

or equivalently

$$\int_b^\infty P(Y_r \le t)\ rdr = \mathscr{L}^{-1}\left[\frac{\hat{\xi}\,(b,s)}{s\ 2\pi\rho}\right]\ . \tag{4.2.11}$$

Therefore (4.2.9) becomes

$$\lim_{\substack{N\to\infty \\ a\to\infty}} P(T_N > t) = e^{-\mathscr{L}^{-1}\left[\frac{\hat{\xi}(b,s)}{s}\right]}$$

$$= e^{-\int_0^t \xi(b,x)\ dx} \tag{4.2.12}$$

$\xi(b,x)$ is numerically tabulated in Jaeger (1943) and decreases monotonically to 0. Hence (4.2.12) is an example of a distribution with a decreasing hazard rate, DHR.

Let T_{iN} be the time for i–th collision, and define $G_{iN}(t) = P(T_{iN} \le t)$. Denote $Q = P(\tau \le t) = \frac{2\pi\rho}{N} \int_b^\infty P(Y_r \le t)\, rdr$, then the probability density $g_{iN}(t)$ of T_{iN} can be expressed as:

$$g_{iN}(t) = \frac{N!}{(i-1)!(N-i)!} Q^{i-1} (1-Q)^{N-i} \frac{dQ}{dt} \quad \text{for } i \ge 1 \tag{4.2.13}$$

where Q^{i-1} corresponds to probability of i–1 particles with $\tau < t$ and $(1-Q)^{N-i}$ corresponds to probability of N–i particles with $\tau > t$.

From (4.2.11) we have

$$\int_0^t \xi(b,x)\, dx = 2\pi\rho \int_b^\infty P(Y_r \le t)\, rdr = NQ,$$

(4.2.13) becomes

$$g_{iN}(t) = \frac{1}{(i-1)!} \left[\int_0^t \xi(b,x)\, dx\right]^{i-1} e^{-\int_0^t \xi(b,x)dx} \xi(b,t). \tag{4.2.14}$$

4.3 n–DIMENSIONAL HITTING PROBABILITIES

N points are randomly scattered in the region $b < r \le a$ of R^n such that the distribution of the number of points in any volume is a Poisson distribution. An n–sphere of radius b is centred at the origin. One wishes to determine the distribution of first and i–th collision time on the central sphere under the assumption that the points are executing free Brownian motion.

Let $V_n(r)$ and $A_n(r)$ be the volume and surface content of an n–sphere of radius r, then

$$V_n(r) = C_n\ r^n,\ A_n(r) = nC_n\ r^{n-1}$$

where $C_n = \dfrac{2\pi^{n/2}}{n\Gamma\left[\frac{n}{2}\right]}$ and $\Gamma(n)$ is the gamma function.

Following a similar argument as in two dimensions.

Denote Y_R be the first hitting time of a Brownian particle with initial distance R from the centre of the n–sphere. The point P_1 under consideration was randomly placed within the region $b < r \leq a$, such that the density function of it's distance to the origin is:

$$f(r) = \begin{cases} \dfrac{nC_n\ r^{n-1}}{C_n\ (a^n - b^n)} & b < r \leq a \\ 0 & \text{otherwise.} \end{cases} \tag{4.3.1}$$

Define τ be the time for P_1 hits the inner n–sphere, then

$$P(\tau \leq t) = \int_b^\infty P(Y_r \leq t)\ \frac{n\ C_n\ r^{n-1}}{a^n - b^n}\ dr \tag{4.3.2}$$

(4.3.2) can be written as:

$$P(\tau \leq t) = \frac{n\rho C_n}{N} \int_b^a P(Y_r \leq t)\ r^{n-1}\ dr$$

where ρ is the density of particles in the region $b < r \leq a$

$$\left[\text{i.e. } \rho = \frac{N}{C_n(a^n - b^n)}\right].$$

Let T_N be the time of first hit, we have

$$P(T_N > t) = [1 - P(\tau \le t)]^N$$

$$= \left[1 - \frac{n\rho C_n}{N} \int_b^a P(Y_r \le t)\, r^{n-1}\, dr\right]^N$$

$$\lim_{\substack{N\to\infty \\ a\to\infty}} P(T_N > t) = e^{-n\rho C_n \int_b^\infty P(Y_r \le t)\, r^{n-1}\, dr}. \tag{4.3.3}$$

Now

$$\mathscr{L}\left[\int_b^\infty P(Y_r \le t)\, r^{n-1}\, dr\right] = \int_0^\infty e^{-st} \int_b^\infty P(Y_r \le t)\, r^{n-1}\, drdt$$

$$= \frac{1}{s} \int_b^\infty r^{n-1}\, E\left[e^{-sY_r}\right] dr. \tag{4.3.4}$$

From John Kent (1978), we have

$$E\left[e^{-sYr}\right] = \left[\frac{b}{r}\right]^\nu \frac{K_\nu\left[\sqrt{\frac{s}{D}}\, r\right]}{K_\nu\left[\sqrt{\frac{s}{D}}\, b\right]} \text{ where } \nu = \frac{n-2}{2}. \tag{4.3.5}$$

Putting (4.3.5) into (4.3.4), we have

$$\mathscr{L}\left[\int_b^\infty P(Y_r \le t)\, r^{n-1}\, dr\right] = \frac{b^\nu}{s\left[K_\nu\left[\sqrt{\frac{s}{D}}\, b\right]\right]} \int_b^\infty r^{n-1-\nu}\, K_\nu\left[\sqrt{\frac{s}{D}}\, r\right] dr. \quad (4.3.6)$$

But

$$\int_b^\infty r^{n-1-\nu} K_\nu\left[\sqrt{\frac{s}{D}}\, r\right] dr = \int_0^\infty r^{\frac{n}{2}}\, K_{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\, r\right] dr - \int_0^b r^{\frac{n}{2}}\, K_{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\, r\right] dr. \quad (4.3.7)$$

Using the identities (see Gradshteyn & Ryzik, p.683, p.685):

$$\int_0^\infty x^\mu\, K_\nu(ax)\, dx = 2^{\mu-1}\, a^{-\mu-1}\, \Gamma\left[\frac{1+\mu+\nu}{2}\right] \Gamma\left[\frac{1+\mu-\nu}{2}\right]$$

and

$$\int_0^1 x^{\nu+1}\, K_\nu(ax)\, dx = 2^\nu\, a^{-\nu-2}\, \Gamma(\nu+1) - a^{-1}\, K_{\nu+1}(a),$$

we obtain

$$\int_0^\infty r^{\frac{n}{2}} K_{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\, r\right] dr = 2^{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\, r\right]^{-\frac{n}{2}-1} \Gamma\left[\frac{1+\frac{n}{2}+\frac{n}{2}-1}{2}\right]\cdot\Gamma\left[\frac{1+\frac{n}{2}-\frac{n}{2}+1}{2}\right]$$

$$= 2^{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\right]^{-\frac{n}{2}-1} \Gamma\left[\frac{n}{2}\right] \quad (4.3.8)$$

and

$$\int_0^b r^{\frac{n}{2}} K_{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\, r\right] dr = b \int_0^1 (ub)^{\frac{n}{2}} K_{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\, ub\right] du$$

$$= b^{1+\frac{n}{2}} \int_0^1 u^{\frac{n}{2}} K_{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\, bu\right] du$$

$$= b^{1+\frac{n}{2}}\left[2^{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\, b\right]^{-\frac{n}{2}+1-2} \Gamma\left[\frac{n}{2}\right] - \left[\sqrt{\frac{s}{D}}\, b\right]^{-1} K_{\frac{n}{2}}\left[\sqrt{\frac{s}{D}}\, b\right]\right]. \tag{4.3.9}$$

Putting (4.3.8), (4.3.9) into (4.3.7), we have

$$\int_b^{\infty} r^{n-1-\nu} K_{\nu}\left[\sqrt{\frac{s}{D}}\, r\right] dr = \left[\sqrt{\frac{s}{D}}\, b\right]^{-1} b^{\frac{n}{2}+1} K_{\frac{n}{2}}\left[\sqrt{\frac{s}{D}}\, b\right]$$

hence

$$\mathscr{L}\left[\int_b^{\infty} P(Y_r \leq t)\, r^{n-1}\, dr\right] = \frac{b^{n-1}}{s}\sqrt{\frac{D}{s}}\, \frac{K_{\frac{n}{2}}\left[\sqrt{\frac{s}{D}}\, b\right]}{K_{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\, b\right]} = \frac{\hat{\xi}(b,s)}{snC_n\rho}$$

where

$$\hat{\xi}(b,s) = nC_n\, b^{n-1}\, D\, \frac{\rho}{s}\sqrt{\frac{s}{D}}\, \frac{K_{\frac{n}{2}}\left[\sqrt{\frac{s}{D}}\, b\right]}{K_{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\, b\right]} \text{ (from 4.1.8).}$$

Therefore

$$\lim_{\substack{N\to\infty \\ a\to\infty}} P(T_N > t) = e^{-\mathscr{L}^{-1}\left[\frac{\hat{\xi}(b,s)}{s}\right]} = e^{-\int_0^t \xi(b,x)dx}. \tag{4.3.10}$$

Again, it is a distribution with a decreasing hazard rate DHR. The density function of i–th collision time on the central n–sphere is identical to (4.2.14) except

$$\hat{\xi}(b,s) = \rho\, nC_n\, b^{n-1} \sqrt{\frac{D}{s}}\, \frac{K_{\frac{n}{2}}\left[\sqrt{\frac{s}{D}}\, b\right]}{K_{\frac{n}{2}-1}\left[\sqrt{\frac{s}{D}}\, b\right]}\,.$$

Define a random variable T such that $T = T_N$ when $n \to \infty$ and $a \to \infty$,

i.e.
$$\lim_{\substack{N\to\infty \\ a\to\infty}} T_N = T.$$

The moment generating function of T is calculated for $n = 3$.

If $n = 3$,

$$\hat{\xi}(b,s) = 4\pi b^2 \rho \sqrt{\frac{D}{s}}\, \frac{K_{\frac{3}{2}}\left[\sqrt{\frac{s}{D}}\, b\right]}{K_{\frac{1}{2}}\left[\sqrt{\frac{s}{D}}\, s\right]}\,.$$

Since (see Watson page 80)

$$K_{n+\frac{1}{2}}(x) = \left[\frac{\pi}{2x}\right]^{\frac{1}{2}} e^{-x} \sum_{r=0}^{n} \frac{(n+r)!}{r!\,(n-r)!\,(2x)^r}$$

we have

$$\hat{\xi}(b,s) = 4\pi b^2 \rho \sqrt{\frac{D}{s}} \left[1 + \sqrt{\frac{D}{s}}\,\frac{1}{b}\right]$$

or

$$\xi(b,t) = 4\pi\rho b D \left[\frac{b}{\sqrt{\pi D t}} + 1\right].$$

Therefore

$$P(T > t) = e^{-\int_0^t 4\pi\rho bD\left[\frac{b}{\sqrt{\pi Dx}} + 1\right]dx}$$

and the probability density function f(t) of T:

$$f(t) = 4\pi\rho bD \left[1 + \frac{b}{\sqrt{\pi Dt}}\right] e^{-4\pi\rho bD\left[t + \frac{2b\sqrt{t}}{\sqrt{\pi D}}\right]} .$$

The moment generating function $\mathscr{E}(e^{-sT})$ of T becomes:

$$\mathscr{E}(e^{-sT}) = \int_0^\infty e^{-st} f(t)dt$$

$$= 4\pi\rho bD \int_0^\infty \left[1 + \frac{b}{\sqrt{\pi Dt}}\right] e^{-4\pi\rho bD\left[t + \frac{2b\sqrt{t}}{\sqrt{\pi D}}\right]} e^{-st}\, dt.$$

Using integral table (Gröbner and Hofreiter) and change of variables, we have

$$\mathscr{E}(e^{-sT}) = 8\pi\rho bD\left\{\frac{1}{2(s+4\pi\rho bD)} - \frac{e^{\frac{16\rho^2 b^4 \pi D}{s+4\pi\rho bD}}}{s+4\pi\rho bD}\left[\frac{\sqrt{\pi}}{2}\left[1- \operatorname{erf}\left[\frac{4\rho b^2\sqrt{\pi D}}{\sqrt{s+4\pi\rho bD}}\right]\right]\right] \frac{4\rho b^2\sqrt{\pi D}}{\sqrt{s+4\pi\rho bD}}\right.$$

$$\left. + \frac{b}{\sqrt{\pi D}}\,\frac{1}{2}\sqrt{\frac{\pi}{s+4\pi\rho bD}}\; e^{\frac{16\rho^2 b^4 \pi D}{s+4\pi\rho bD}} \left[1- \operatorname{erf}\left[\frac{4\rho b^2\sqrt{\pi D}}{\sqrt{s+4\pi\rho bD}}\right]\right]\right\}$$

$$= 8\pi\rho bD\left\{\frac{1}{2(s+4\pi\rho bD)}+\frac{bs}{2\sqrt{D}(s+4\pi\rho bD)^{3/2}} \left[1-\operatorname{erf}\left[\frac{4\rho b^2\sqrt{\pi D}}{\sqrt{s+4\pi\rho bD}}\right]\right] e^{\frac{16\rho^2 b^4 \pi D}{s+4\pi\rho bD}}\right\} \quad (4.3.11)$$

where $\mathrm{erf}(t) = \frac{2}{\sqrt{\pi}} \int_0^t e^{-x^2}\, dx.$

Using $\mathrm{erf}(t) = -1 + 2\,\Phi(\sqrt{2}\, t)$

where $\Phi(x)$ is the cumulative distribution for standard Normal distribution, i.e.

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{\frac{-y^2}{2}}\, dy$$

(4.3.11) can be expressed as

$$\mathscr{E}(e^{-sT}) = 8\pi\rho bD\Big\{\frac{1}{2(s+4\pi\rho bD)} + \frac{bs}{\sqrt{D}(s+4\pi\rho bD)^{3/2}}\left[1-\Phi\left[\frac{4\sqrt{2}\rho b^2\sqrt{\pi D}}{\sqrt{s+4\pi\rho bD}}\right]\right] e^{\frac{16\rho^2 b^4 \pi D}{s+4\pi\rho bD}}\Big\}. \quad (4.3.12)$$

Hence the mean time μ for the first absorption of points is:

$$\mu = -\frac{\partial}{\partial s}\mathscr{E}(e^{-sT})\Big|_{s=0} = \frac{1}{4\pi\rho bD} - \frac{e^{4\rho b^3}}{D}\sqrt{\frac{b}{\pi\rho}}\,(1 - \Phi(\sqrt{8\rho b}\; b))$$

With diffusion coefficient $D = 0.5\ \mathrm{cm}^2/\mathrm{s}$, the mean first hitting time for 3 dimension is plotted in figure 4.1 for different values of radius and density.

Figure 4.1 indicates that the expected first hitting time (a) decreases with the size of central sphere and (b) decreases with the density of the points.

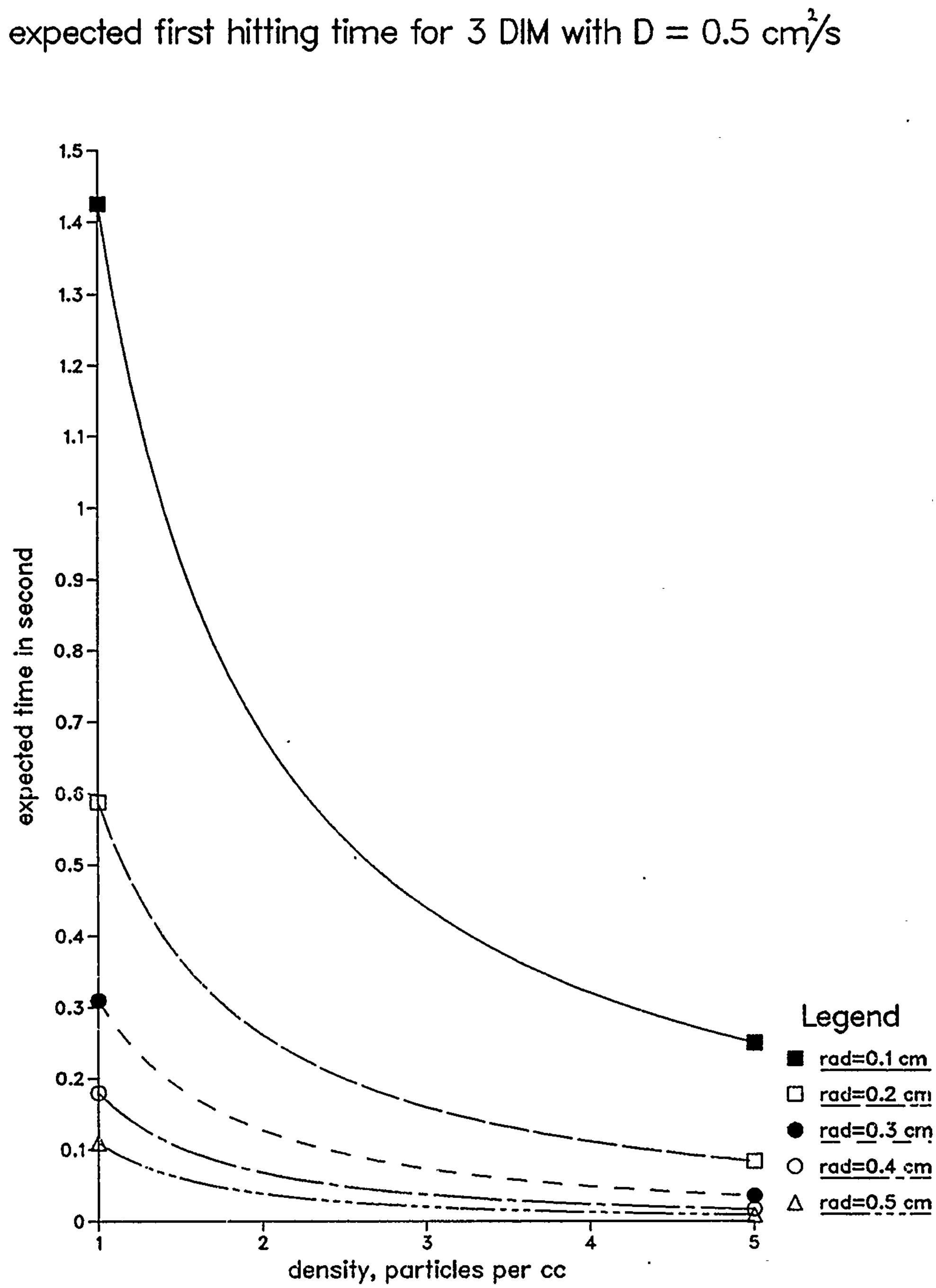

expected first hitting time for 3 DIM with D = 0.5 cm²/s
expected time in second
density, particles per cc
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1
2
3
4
5
Legend
rad=0.1 cm
rad=0.2 cm
rad=0.3 cm
rad=0.4 cm
rad=0.5 cm

Figure 4.1

Next, we want to determine the probability $P\{Y_R < \infty\}$ where $R > b$. But

$$P\{Y_R < \infty\} = \lim_{s \downarrow 0} E(e^{-sY_R})$$

From (4.3.5), we have

$$P\{Y_R < \infty\} = \lim_{s \downarrow 0} \left[\frac{b}{R}\right]^{\nu} \frac{K_\nu\left[\sqrt{\frac{s}{D}}\, R\right]}{K_\nu\left[\sqrt{\frac{s}{D}}\, b\right]} \text{ where } \nu = \frac{n-2}{2}. \tag{4.3.13}$$

Since $K_\nu(x) \sim \frac{\Gamma(\nu)}{2} \left[\frac{x}{2}\right]^{-\nu}$ as $x \to 0$, for $\nu > 0$ (4.3.13) can be written as:

$$P\{Y_R < \infty\} = \left[\frac{b}{R}\right]^{\frac{n-2}{2}} \left\{\frac{\Gamma\left[\frac{n-2}{2}\right]}{2} \left[\frac{\sqrt{\frac{s}{D}}\, R}{2}\right]^{-\frac{n-2}{2}}\right\} \left\{\left[\frac{\Gamma\left[\frac{n-2}{2}\right]}{2}\right]^{-1} \cdot \left[\frac{\sqrt{\frac{s}{D}}\, b}{2}\right]^{\frac{n-2}{2}}\right\}$$

$$= \left[\frac{b}{R}\right]^{n-2} \qquad \forall\, n > 2. \tag{4.3.14}$$

For $n = 2$, from (4.2.5), we have

$$P\{Y_R < \infty\} = \lim_{s \to 0} \frac{K_0\left[\sqrt{\frac{s}{D}}\, R\right]}{K_0\left[\sqrt{\frac{s}{D}}\, b\right]}.$$

Since $K_0(x) \sim -\log x$, as $x \to 0$, we have

$$P\{Y_R < \infty\} = \lim_{s \to 0} \frac{\log\left[\sqrt{\frac{s}{D}}\, R\right]}{\log\left[\sqrt{\frac{s}{D}}\, b\right]}. \tag{4.3.15}$$

By L'Hopital rule, (4.3.15) can be written as:

$$P\{Y_R < \infty\} = \lim_{s \to 0} \frac{\frac{d}{ds} \log\left[\sqrt{\frac{s}{D}}\, R\right]}{\frac{d}{ds} \log\left[\sqrt{\frac{s}{D}}\, b\right]} = 1 \qquad (4.3.16)$$

i.e. the point will always hit the circle.

In free Brownian motions in one dimension there is probability one that the particle will sooner or later hit the origin. In two dimensions, there is probability one that the particle with initial distance R from the origin will sooner or later hit the central circle of radius b with $b < R$. For dimension $n \geq 3$, the probability of hitting the central n–sphere will be $\left[\frac{b}{R}\right]^{n-2}$. i.e.

$$P\{R(t) \leq b \mid R(0) = R \text{ for some } t > 0\} = \left[\frac{b}{R}\right]^{n-2},\ n \geq 3.$$

Kakutani (1944) used a completely different approach to obtain the probability of $\frac{b}{R}$ for three dimensions. For $n \geq 3$ dimensions, one can find egn. (4.3.14) in Port and Stone's (1978) page 56.

CHAPTER V

BROWNIAN MOTION WITHIN A VIEWING FIELD

5.1 INTRODUCTION:

If a particle undergoing Brownian motion is selected at random from a region E in $\mathbb{R}^n$, then what is the probability that the particle will be in a convex region G in $\mathbb{R}^n$ a time t later, where $E \subset G$. For example, one may select a particle while viewing cells under a microscope and ask the probability that the particle will be in the viewing field a time t later. We will consider particles that may leave the viewing field but return before time t. If a particle is selected at time $t = 0$, then define the random variable R_t as the distance of the particle from its starting position a time t later. Then we have $G_t(r) = P\{R_t < r\}$ and $g_t(r) = \frac{dG_t(r)}{dr}$.

A particle is now chosen at random from E in $\mathbb{R}^n$ and observed again a time t later. Then define:

$$Q_{E,G}(t) = P\{\text{particle chosen randomly in E is in G a time t later}\}$$

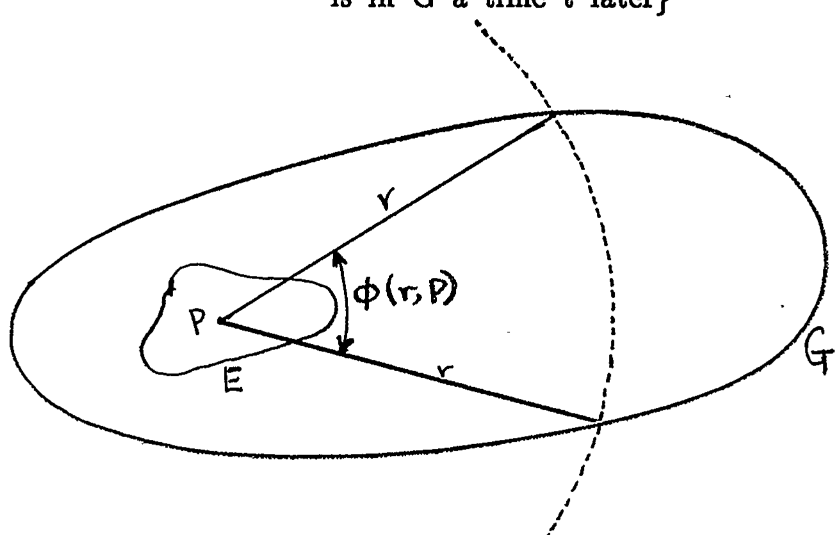


Figure 5.1

Let P be the random point chosen in E. Then surround P with an n–dimensional spherical shell of radius r, see Figure 5.1. Then the probability that the particle is in G when it has moved a net distance of $R_t = r$ is related to the angle $\phi(r,P)$ subtended by the spherical shell in G, namely

$$Q_{E,G}(t|P) = \int_0^\infty g_t(r) \frac{\phi(r,P)}{nC_n} dr \tag{5.1.1}$$

where nC_n is the total solid angle in $\mathbb{R}^n$. We have used the fact that Brownian motion is spherically symmetric, hence the likelihood of a particle being in any given solid angle is the same as in any other solid angle of the same magnitude.

The using results (1.1) and (2.3) from Enns and Ehlers (1988), one may write:

$$\begin{aligned} \Omega_{E,G}(\ell) &= \mathscr{E}_{P_E}\left[\frac{\phi(\ell,P)}{nC_n}\right] \\ &= \mathscr{E}_\theta[V(E(\ell,\theta)\cap G)]/V(E) \end{aligned} \tag{5.1.2}$$

where $\mathscr{E}_{P_E}(\cdot)$ is the expected value of $(\cdot)$ when P is uniformly averaged over the region E. Similarly $E(\ell,\theta)$ is the region E translated a distance ℓ in direction θ and the translated overlap volume with G is uniformly averaged over all possible directions.

Equation (5.1.1) may then be rewritten as

$$Q_{E,G}(t) = \mathscr{E}_{P_E}\left[Q_{E,G}(t|P)\right] = \int_0^\infty g_t(r)\ \Omega_{E,G}(r)\ dr \tag{5.1.3}$$

Now also from Enns and Ehlers (1988), one defines a ν–random ray as the line segment from a point P chosen randomly and uniformly in $E \subset G$ to the boundary of G where the direction of the ray is randomly generated from all possible directions. Then the length of this ray S satisfies:

$$P(S \geq \ell) = \bar{F}(\ell) = \Omega_{E,G}(\ell) \tag{5.1.4}$$

with p.d.f. $f(\ell) = -\, d\Omega_{E,G}(\ell)\ /d\ell$.

An integration by parts yields alternative versions of (5.1.3) as:

$$\begin{aligned} Q_{E,G}(t) &= \int_0^\infty G_t(r)\ f(r)\ dr \\ &= \mathscr{E}[G_t(S)], \text{ where the expectation is with respect to the measure } \nu. \\ &= P\{R_t < S\}. \end{aligned} \tag{5.1.5}$$

Below, $Q_{E,G}(t)$ is calculated for the following cases:

(a) $E = G$, disc or ball and (b) $E \subset G$, concentric balls.

5.2 DISC WITH E = G

At time $t = 0$, the particle considered is at origin 0 and executes free Brownian Motion with diffusion coefficient D. Let $W_t(x,y)$ be the probability density that a particle reaches (x,y) in the time t. Then

$$W_t(x,y) = \frac{1}{4\pi Dt}\, e^{-\frac{(x^2+y^2)}{4Dt}}$$

which satisfies the diffusion equation:

$$\frac{\partial}{\partial t} W_t(x,y) = D\nabla^2 W_t = D\left[\frac{\partial^2}{\partial x^2} W_t + \frac{\partial^2}{\partial y^2} W_t\right].$$

Since what interests us is the distance of the particle from the centre of diffusion, origin O, it is more convenient to convert to polar co–ordinates.

Let $x = r\cos\theta$, $y = r\sin\theta$, then $dxdy = rdrd\theta$ and in polar form, $W_t(x,y)$ can be expressed as:

$$W_t(x,y)\ dxdy = W_t(r,\theta)\ \ rdrd\theta$$

$$= \frac{1}{4\pi Dt}\, r\, e^{-\frac{r^2}{4Dt}}\ drd\theta.$$

Therefore

$$P\{R(t) < r \mid r(0) = 0\} = \frac{1}{4\pi Dt}\int_0^{2\pi}\int_0^{r} r_1\, e^{-\frac{r_1^2}{4Dt}}\ dr_1 d\theta$$

$$= \frac{1}{2Dt}\int_0^{r} e^{-\frac{r_1^2}{4Dt}}\ r_1 dr_1 = 1 - e^{-\frac{r^2}{4Dt}}. \tag{5.2.1}$$

Denote $P\{R(t) < r \mid r(0) = 0\}$ by $G_t(r)$, hence

$$G_t(r) = 1 - e^{-\frac{r^2}{4Dt}} \tag{5.2.2}$$

and the probability density (Karlin and Taylor (1974) page 370)

$$g_t(r) = \frac{\partial}{\partial r} G_t(r) = \frac{r}{2Dt}\, e^{-\frac{r^2}{4Dt}}\ . \tag{5.2.3}$$

Using equation (5.1) in Enns and Ehlers (1988), putting E = G (i.e. b = a), and for n dimension, we have

$$\Omega(r) = \begin{cases} 2\,\dfrac{C_{n-1}}{C_n}\displaystyle\int_0^{\alpha} \sin^n \theta \, d\theta & 0 \leq r \leq 2a \\ 0 & \text{otherwise} \end{cases} \tag{5.2.4}$$

where $\cos\alpha = \frac{r}{2a}$ and $C_n = \dfrac{2\pi^{n/2}}{n\Gamma\left[\frac{n}{2}\right]}$.

$\Omega(r)$ may also be expressed as

$$\Omega(r) = \begin{cases} 2\,\dfrac{C_{n-1}}{C_n}\displaystyle\int_{\frac{r}{2a}}^{1} (1-u^2)^{\frac{n-1}{2}} \, du & 0 \leq r \leq 2a \\ 0 & \text{otherwise.} \end{cases} \tag{5.2.5}$$

Hence for n = 2, we have

$$\Omega(r) = \frac{4}{\pi}\int_{\frac{r}{2a}}^{1} (1-u^2)^{\frac{1}{2}} \, du$$

and therefore, using 5.1.4,

the probability density for the ray R, is:

$$f_R(r) = \begin{cases} \dfrac{1}{\pi a^2}\sqrt{4a^2-r^2} & 0 \leq r \leq 2a \\ 0 & \text{otherwise .} \end{cases} \tag{5.2.6}$$

$$Q_E(t) = \int_0^{\infty} G_t(r) \cdot f_R(r) \cdot dr$$

$$= \int_0^{2a} \left[1 - e^{-\frac{r^2}{4Dt}}\right] \frac{\sqrt{4a^2 - r^2}}{\pi a^2}\, dr$$

$$= \frac{1}{\pi a^2}\left[\int_0^{2a} \sqrt{4a^2-r^2}\, dr - \int_0^{2a} e^{-\frac{r^2}{4Dt}} \sqrt{4a^2-r^2}\, dr\right]. \tag{5.2.7}$$

Write $I_1 = \int_0^{2a} \sqrt{4a^2-r^2}\, dr$ and $I_2 = \int_0^{2a} e^{-\frac{r^2}{4Dt}} \sqrt{4a^2-r^2}\, dr.$

and let

$r = 2a \sin \theta$, $dr = 2a \cos \theta \, d\theta$. Then we have

$$I_1 = 4a^2 \int_0^{\pi/2} \cos^2 \theta \, d\theta = 2a^2 \left[\theta + \frac{\sin 2\theta}{2}\bigg|_0^{\pi/2}\right]$$

$$= \pi a^2, \tag{5.2.8}$$

while

$$I_2 = 4a^2 \int_0^{\pi/2} e^{-\frac{a^2 \sin^2\theta}{Dt}} \cos^2\theta d\theta$$

$$= 4a^2 \left[\int_0^{\pi/2} e^{-\frac{a^2 \sin^2\theta}{Dt}} d\theta - \int_0^{\pi/2} e^{-\frac{a^2 \sin^2\theta}{Dt}} \sin^2\theta d\theta\right]$$

$$= 4a^2 \left[\sum_{i=0}^{\infty} \frac{(-1)^i}{i!} \left[\frac{a^2}{Dt}\right]^i \int_0^{\pi/2} \sin^{2i}\theta d\theta - \sum_{i=0}^{\infty} \frac{(-1)^i}{i!} \left[\frac{a^2}{Dt}\right]^i \int_0^{\pi/2} \sin^{2(i+1)}\theta d\theta \right].$$

Using $\int_0^{\pi/2} \sin^{2m}\theta d\theta = \frac{\sqrt{\pi}}{2} \frac{\Gamma(m+\frac{1}{2})}{m!}$, then we have

$$I_2 = 4a^2 \left[\sum_{i=0}^{\infty} \frac{(-1)^i}{i!} \left[\frac{a^2}{Dt}\right]^i \frac{\sqrt{\pi}}{2} \frac{\Gamma(i+\frac{1}{2})}{i!} - \sum_{i=0}^{\infty} \frac{(-1)^i}{i!} \left[\frac{a^2}{Dt}\right]^i \frac{\sqrt{\pi}}{2} \frac{\Gamma(i+\frac{3}{2})}{(i+1)!} \right]$$

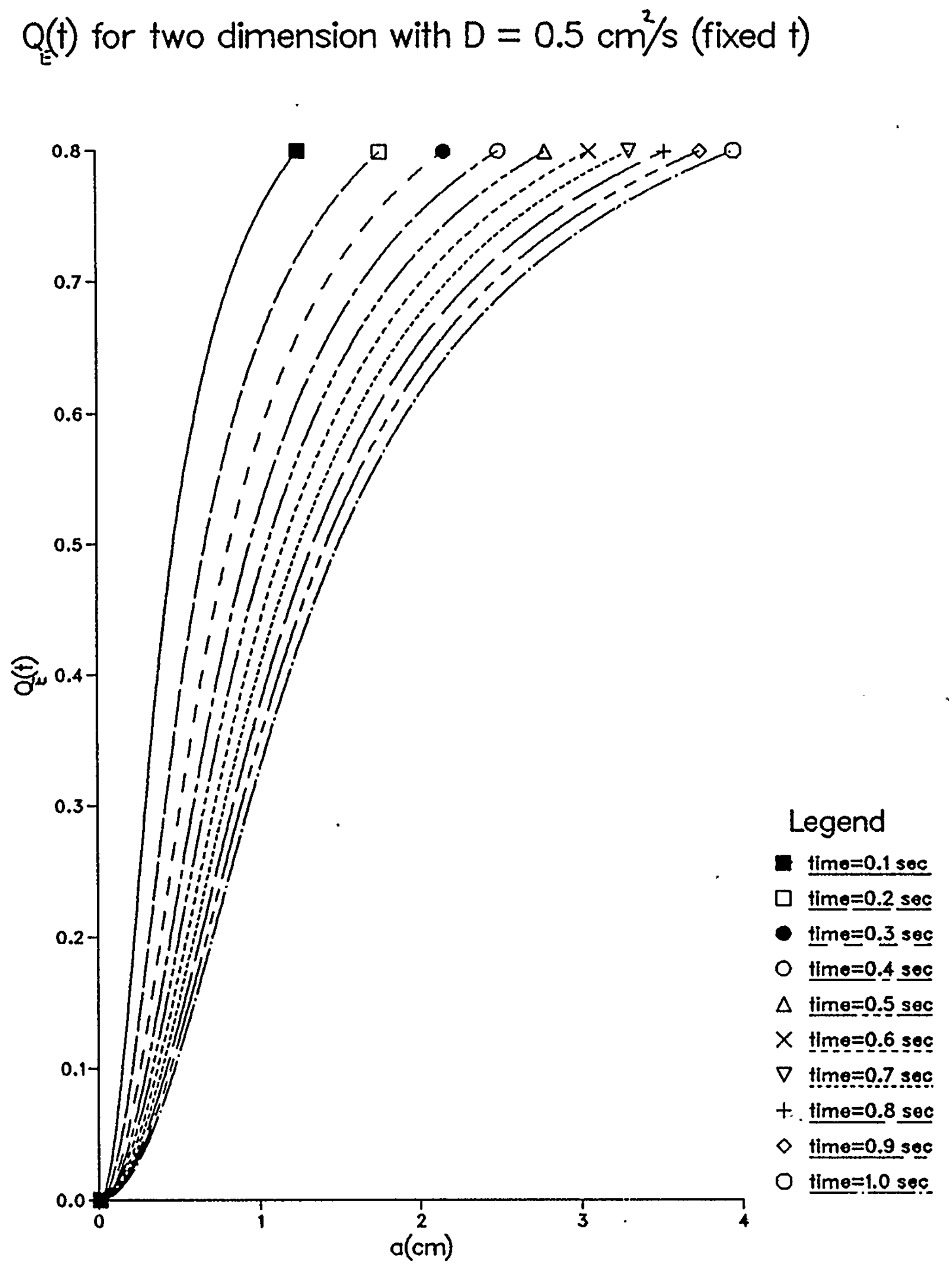
$$= \sqrt{\pi}\, a^2 \left[\sum_{i=0}^{\infty} \frac{(-1)^i}{i!} \left[\frac{a^2}{Dt}\right]^i \frac{\Gamma(i+\frac{1}{2})}{(i+1)!} \right]. \tag{5.2.9}$$

By putting (5.2.9), (5.2.8) into (5.2.7), we have

$$Q_E(t) = \frac{1}{\sqrt{\pi}} \sum_{i=1}^{\infty} \frac{(-1)^{i+1}\ \Gamma(i+\frac{1}{2})}{i!\,(i+1)!} \left[\frac{a^2}{Dt}\right]^i . \tag{5.2.10}$$

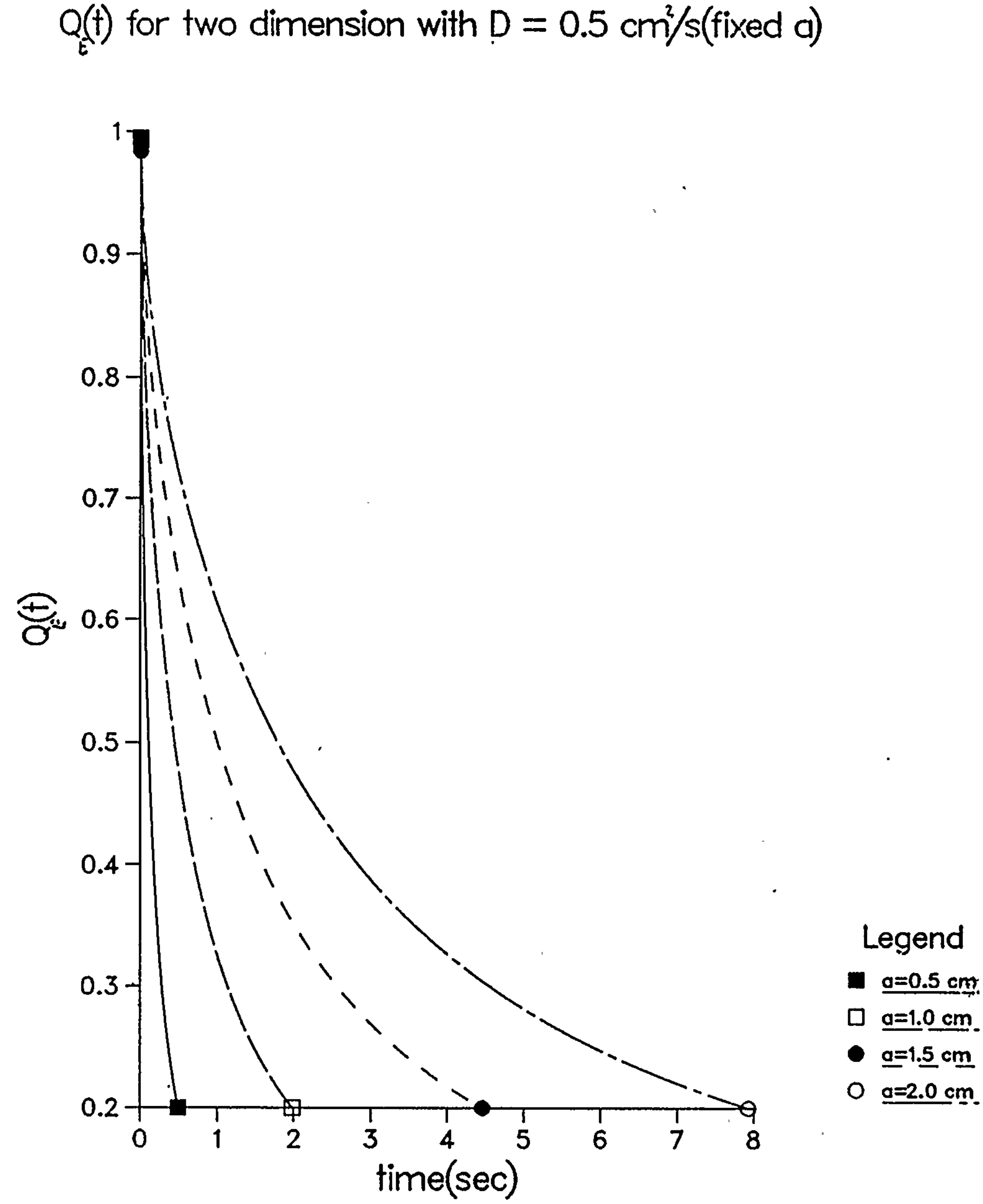
Numerical integration is required to evaluate $Q_E(t)$ in eqn. (5.2.7). For a given time t, the graph of $Q_E(t)$ versus radius a is plotted in Figure 5.2. For a given radius a, the graph of $Q_E(t)$ versus time t is plotted in Figure 5.3.

Both graphs indicate that (a) $Q_E(t)$ decreases with time t and (b) $Q_E(t)$ increases with size of viewing field.



Q(t) for two dimension with D = 0.5 cm²/s (fixed t)
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Q(t)
0
1
2
3
4
a(cm)
Legend
time=0.1 sec
time=0.2 sec
time=0.3 sec
time=0.4 sec
time=0.5 sec
time=0.6 sec
time=0.7 sec
time=0.8 sec
time=0.9 sec
time=1.0 sec

Figure 5.2



$Q_\varepsilon(t)$ for two dimension with D = 0.5 cm²/s(fixed a)
$Q_\varepsilon(t)$
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0
1
2
3
4
5
6
7
8
time(sec)
Legend
a=0.5 cm
a=1.0 cm
a=1.5 cm
a=2.0 cm

Figure 5.3

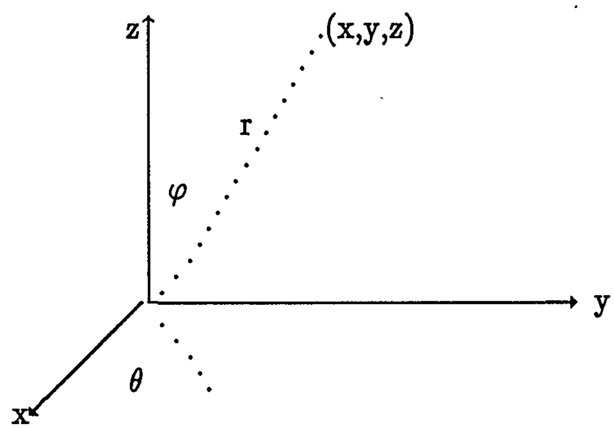
5.3 A SPHERE WITH E = G

The probability density $W_t(x,y,z)$ of a Brownian particle reaching (x,y,z) at time t when it is at the origin 0 at time t = 0 can be expressed as:

$$W_t(x,y,z) = \frac{1}{(4\pi Dt)^{3/2}} e^{-\frac{x^2+y^2+z^2}{4Dt}} .$$

Let $x = r \cos\theta \sin\varphi$, $y = r \sin\theta \sin\varphi$, $z = r \cos\varphi$

(see diagram)



where $0 < \theta < 2\pi$, $0 < \varphi < \pi$, $r > 0$ and the Jacobian $|J| = r^2 \sin\varphi$.

In spherical co-ordinates, we have

$$W_t(x,y,z)\ dxdydz = \frac{1}{(4\pi Dt)^{3/2}} e^{-\frac{r^2}{4Dt}} r^2 \sin\varphi\ drd\theta d\varphi.$$

Integrating over θ and φ, we obtain (Karlin and Taylor (1974) page 368)

$$g_t(r)dr = \frac{4\pi\ r^2 e^{-\frac{r^2}{4Dt}}}{(4\pi Dt)^{3/2}} dr . \tag{5.3.1}$$

Therefore

$$G_t(r) = P\{R(t) < r \mid R(0) = 0\}$$

$$= \frac{4\pi}{(4\pi Dt)^{3/2}} \int_0^r r_1^2 \, e^{\frac{-r_1^2}{4Dt}} \, dr_1$$

$$= \frac{1}{\sqrt{\pi Dt}} \left[\int_0^r e^{\frac{-r_1^2}{4Dt}} \, dr_1 - r \, e^{\frac{-r^2}{4Dt}} \right]. \tag{5.3.2}$$

Putting $n = 3$ in (5.2.4) we have

$$\Omega(r) = \begin{cases} \frac{3}{2} \int_0^{\alpha} \sin^3\theta d\theta & 0 \leq r \leq 2a \\ 0 & \text{otherwise} \end{cases}$$

where $\cos \alpha = \frac{r}{2a}$.

$\Omega(r)$ can also be expressed as:

$$\Omega(r) = \begin{cases} \left[\frac{-r}{2a} + \frac{r^3}{24a^3} + \frac{2}{3}\right] \cdot \frac{3}{2} & 0 \leq r \leq 2a \\ 0 & \text{otherwise} \end{cases} . \tag{5.3.3}$$

$$Q_E(t) = \int_0^{\infty} g_t(r) \; \Omega(r) \; dr$$

$$= \frac{3}{4\sqrt{\pi Dt} \; Dt} \left\{ \int_0^{2a} \frac{r^5}{24a^3} \, e^{\frac{-r^2}{4Dt}} dr - \frac{1}{2a} \int_0^{2a} r^3 \, e^{\frac{-r^2}{4Dt}} dr + \frac{2}{3} \int_0^{2a} r^2 \, e^{\frac{-r^2}{4Dt}} dr \right\} \tag{5.3.4}$$

Let $$I_1 = \int_0^{2a} \frac{r^5}{24a^3}\, e^{-\frac{r^2}{4Dt}} dr$$

$$= \frac{1}{24a^3} \sum_{k=0}^{\infty} \frac{(-1)^k\, 4^{k+3}\, a^{2k+6}}{2(k+3)\; 4^k (Dt)^k k!}$$

$$= \frac{4}{3a^3} \sum_{k=0}^{\infty} \frac{(-1)^k\, a^{2k+6}}{(k+3)\; (Dt)^k\; k!} \; . \tag{5.3.5}$$

Let $$I_2 = -\frac{1}{2a} \int_0^{2a} r^3\, e^{-\frac{r^2}{4Dt}} dr$$

$$= -\frac{4}{a} \sum_{k=0}^{\infty} \frac{(-1)^k\, a^{2k+4}}{(k+2)\; (Dt)^k\; k!} \; . \tag{5.3.6}$$

Let $$I_3 = \frac{2}{3} \int_0^{2a} r^2\, e^{-\frac{r^2}{4Dt}} dr$$

$$= \frac{2}{3} \sum_{k=0}^{\infty} \frac{(-1)^k\, 2^{2k+3}\, a^{2k+3}}{k!\; 4^k\; (Dt)^k\; (2k+3)}$$

$$= \frac{16}{3} \sum_{k=0}^{\infty} \frac{(-1)^k\, a^{2k+3}}{k!\; (Dt)^k\; (2k+3)} \; . \tag{5.3.7}$$

Putting (5.3.5), (5.3.6) and (5.3.7) into (5.3.4), we have

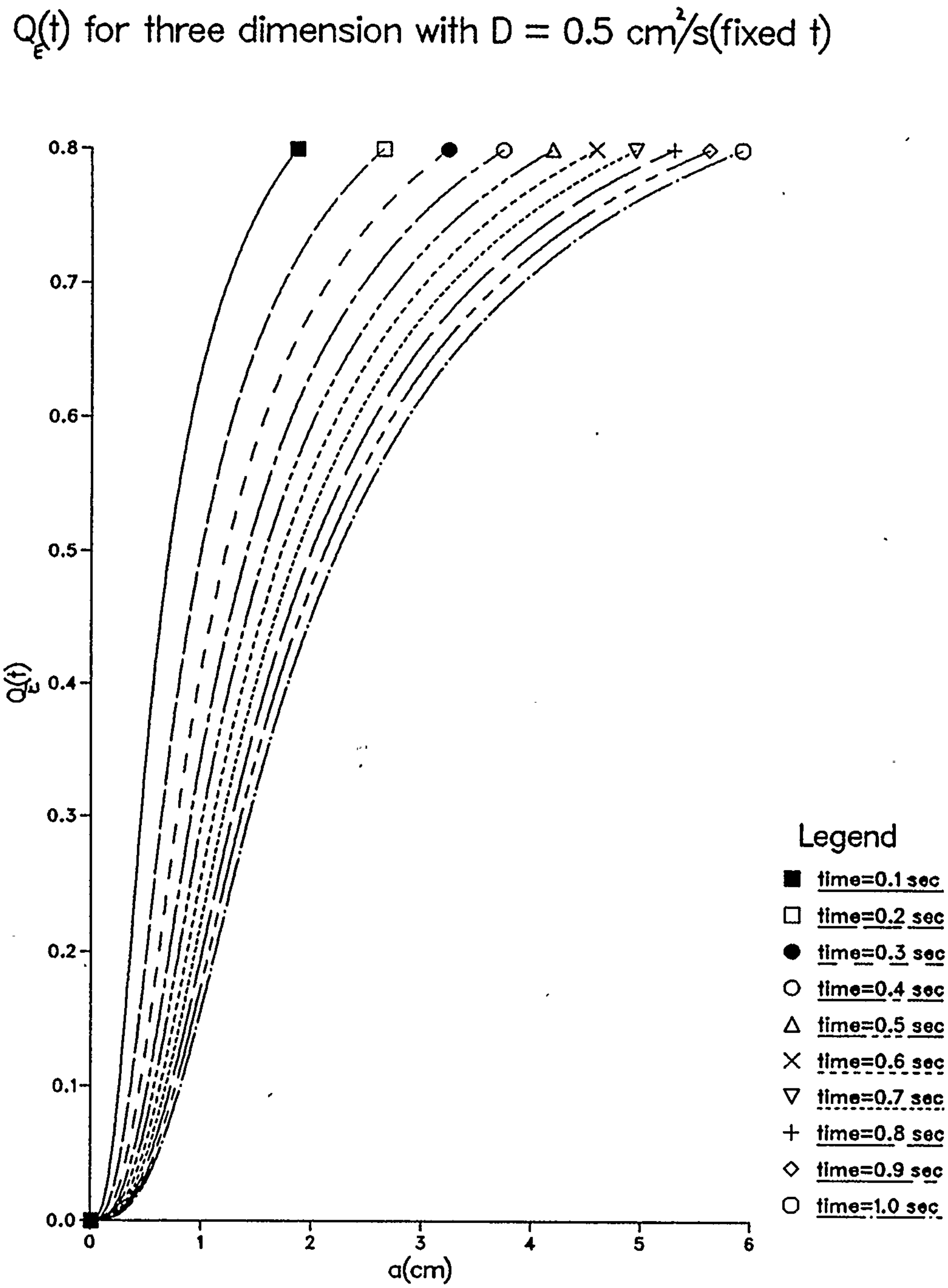
$$Q_E(t) = \frac{3a^3}{Dt\sqrt{\pi Dt}} \sum_{k=0}^{\infty} \frac{(-1)^k a^{2k}}{(2k+3)(k+2)(k+3)(Dt)^k\, k!} . \qquad (5.3.8)$$

Numerical integration is required to evaluate $Q_E(t)$ in eqn.(5.3.4). For a given time, the graph of $Q_E(t)$ versus radius a is plotted in Figure 5.4.
For a given radius a, the graph of $Q_E(t)$ versus time t is plotted in Figure 5.5.

Both graphs (Figure 5.4 and Figure 5.5) indicate that (a) $Q_E(t)$ decreases with time t (b) $Q_E(t)$ increases with the size of viewing field.

Comparison of $Q_E(t)$ between two dimensions and three dimensions is plotted in Figure 5.6 for time fixed at 1.0 second with radius a varying.
Comparison of $Q_E(t)$ between two dimensions and three dimensions is plotted in Figure 5.7 for radius a fixed at 1.0 cm with time t varying.

Both graphs (Figure 5.6, and Figure 5.7) indicate that a particle is more likely to leave the viewing field in three dimensions than in two dimensions due to one extra degree of freedom.



Q_ε(t) for three dimension with D = 0.5 cm²/s(fixed t)
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
Q_ε(t)
0
1
2
3
4
5
6
a(cm)
Legend
time=0.1 sec
time=0.2 sec
time=0.3 sec
time=0.4 sec
time=0.5 sec
time=0.6 sec
time=0.7 sec
time=0.8 sec
time=0.9 sec
time=1.0 sec

Figure 5.4

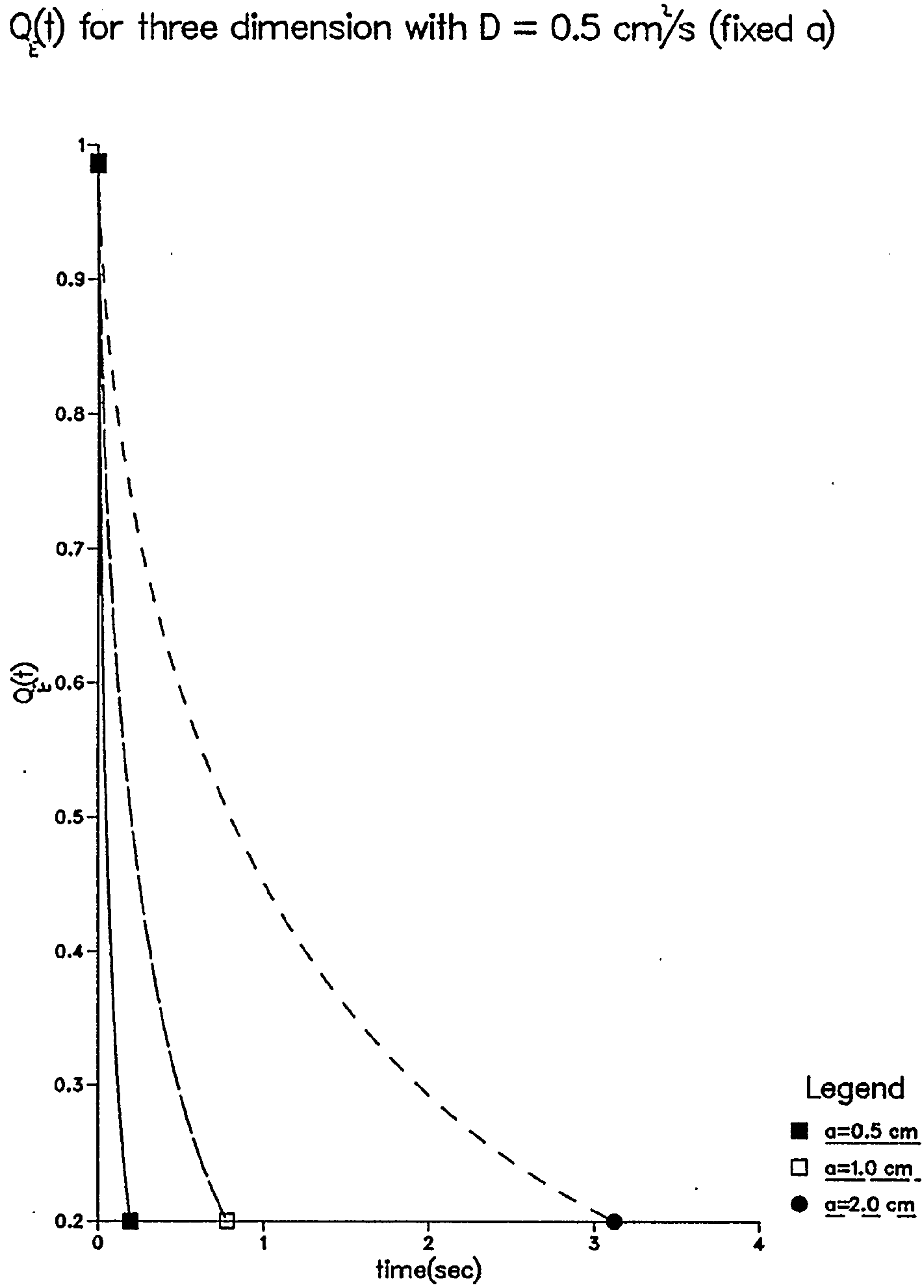

Q(t) for three dimension with D = 0.5 cm²/s (fixed a)
Q(t)
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0
1
2
3
4
time(sec)
Legend
a=0.5 cm
a=1.0 cm
a=2.0 cm

Figure 5.5

$Q_E(t)$ for 2 & 3 dimension with $D = 0.5\ cm^2/s$ and $t=1.0$ sec

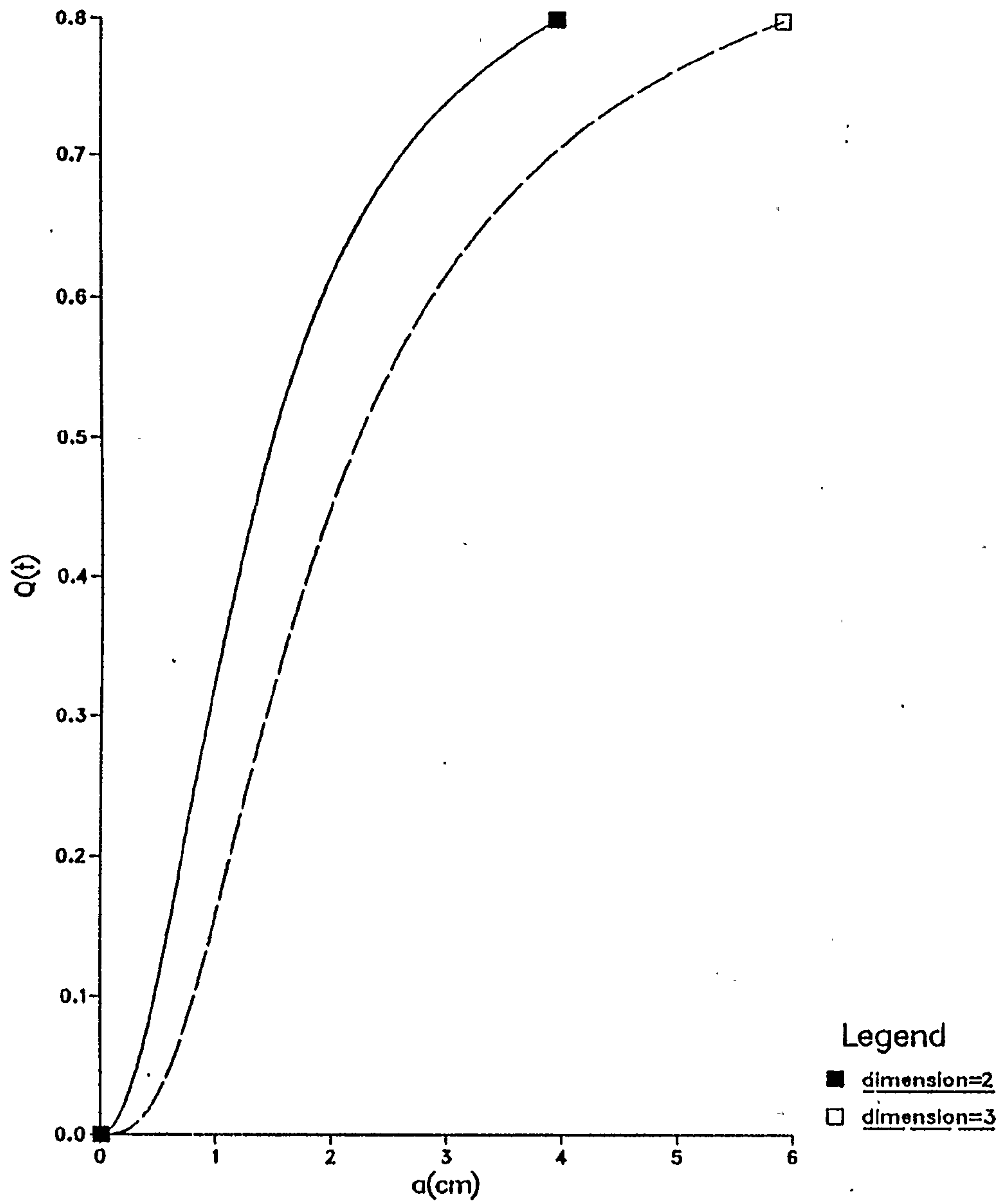


Figure 5.6

$Q_E(t)$ for 2 & 3 dimension with D = 0.5 cm^2/s and a=1.0 cm

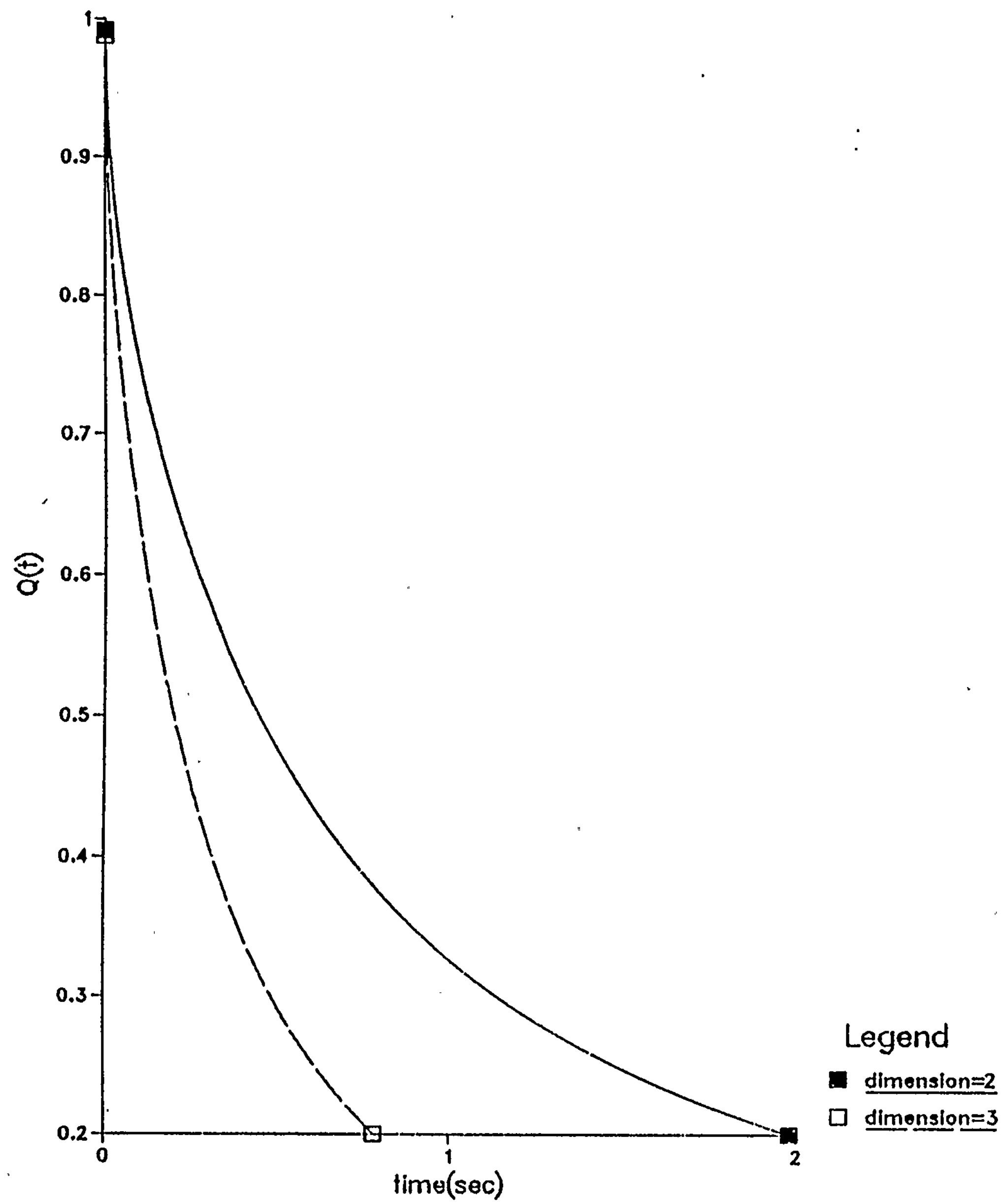


Figure 5.7

5.4 A SPHERE WITH $E \subset G$

From Enns and Ehlers (1988), if E is an n–ball of radius a centered within G, an n–ball of radius of radius b > a, then

$$\Omega_{E,G}(\ell) = \begin{cases} 1 & \text{if } 0 \leq \ell \leq b-a \\ \dfrac{C_{n-1}}{C_n}\left[\displaystyle\int_0^{\alpha} \sin^n\theta d\theta + \left[\frac{b}{a}\right]^n \int_0^{\beta} \sin^n\theta d\theta\right] & \text{if } b-a \leq \ell \leq b+a \\ 0 & \text{if } \ell \geq b+a \end{cases}$$

where $\cos\alpha = \dfrac{\ell^2+a^2-b^2}{2a\ell}$, $\cos\beta = \dfrac{\ell^2+b^2-a^2}{2b\ell}$ and

$$C_n = \frac{2\pi^{n/2}}{n\Gamma\left[\frac{n}{2}\right]} .$$

For n = 3, we have

$$\Omega_{E,G}(\ell) = \begin{cases} 1 & \text{if } 0 \leq \ell \leq b-a \\ \dfrac{3}{4}\left[\displaystyle\int_0^{\alpha} \sin^3\theta d\theta + \left[\frac{b}{a}\right]^3 \int_0^{\beta} \sin^3\theta d\theta\right] & \text{if } b-a \leq \ell \leq b+a. \\ 0 & \text{if } \ell \geq b+a \end{cases}$$

From (5.1.3) and (5.3.1),

$$Q_{E,G}(t) = \int_0^\infty g_t(r)\ \Omega(r)\ dr$$

$$= \frac{4\pi}{(4\pi Dt)^{3/2}} \left\{ \int_0^{b-a} r^2\ e^{-r^2/4Dt}\ dr \right.$$

$$+ \frac{3}{4} \left[\int_{b-a}^{b+a} r^2\ e^{-r^2/4Dt}\ dr \int_0^\alpha \sin^3\ \theta d\theta \right.$$

$$\left. \left. + \left[\frac{b}{a}\right]^3 \int_{b-a}^{b+a} r^2\ e^{-r^2/4Dt}\ dr \int_0^\beta \sin^3\ \theta d\theta \right] \right\} \tag{5.4.1}$$

where $\cos\ \alpha = \dfrac{r^2+a^2-b^2}{2ar}$, $\cos\ \beta = \dfrac{r^2+b^2-a^2}{2br}$.

Denote the first integral on right hand side of (5.4.1) by I_1. Then

$$I_1 = \frac{4\pi}{(4\pi Dt)^{3/2}} \int_0^{b-a} r^2\ e^{-r^2/4Dt}\ dr$$

$$= \frac{1}{2Dt\sqrt{\pi Dt}} \left[-\ 2\ Dt\ (b-a)\ e^{-W_1} + 2\ Dt \sum_{K=0}^{\infty} \frac{(-1)^k\ (b-a)^{2k+1}}{K!\ (4Dt)^k\ (2K+1)} \right]$$

where $W_1 = \dfrac{(b-a)^2}{4Dt}$. (5.4.2)

Denote the second double integral on right hand side of (5.4.1) by I_2, then

$$I_2 = \int_{b-a}^{b+a} r^2\ e^{-r^2/4Dt}\ dr \int_0^\alpha \sin^3\ \theta d\theta.$$

I_2 can be expressed as:

$$I_2 = -\int_{b-a}^{b+a} r^2\, e^{-r^2/4Dt} \left[\frac{r^2+a^2-b^2}{2ar}\right] dr + \frac{1}{3}\int_{b-a}^{b+a} r^2\, e^{-r^2/4Dt} \left[\frac{r^2+a^2-b^2}{2ar}\right]^3 dr$$

$$+ \frac{2}{3}\int_{b-a}^{b+a} r^2\, e^{-r^2/4Dt}\, dr. \tag{5.4.3}$$

Denote the third double integral on right hand side of (5.4.1) by I_3. Then

$$I_3 = \int_{b-a}^{b+a} r^2\, e^{-r^2/4Dt}\, dr \int_0^{\beta} \sin^3 \theta d\theta.$$

Using the same argument as in I_2, we have

$$I_3 = -\int_{b-a}^{b+a} r^2\, e^{-r^2/4Dt} \left[\frac{r^2+b^2-a^2}{2br}\right] dr + \frac{1}{3}\int_{b-a}^{b+a} r^2\, e^{-r^2/4Dt} \left[\frac{r^2+b^2-a^2}{2br}\right]^3 dr$$

$$+ \frac{2}{3}\int_{b-a}^{b+a} r^2\, e^{-r^2/4Dt}\, dr. \tag{5.4.4}$$

From definition of I_1, I_2, I_3, $Q_{E,G}(t)$ can be expressed as:

$$Q_{E,G}(t) = I_1 + \frac{3}{8Dt\sqrt{\pi Dt}} \left[I_2 + \left[\frac{b}{a}\right]^3 I_3\right]. \tag{5.4.5}$$

For the following calculations we write $u_1 = b-a$, $u_2 = b+a$, $W_1 = \frac{u_1^2}{4Dt}$ and

$W_2 = \frac{u_2^2}{4Dt}$. Evaluating the first integral in (5.4.3), we have

$$- \int_{b-a}^{b+a} r^2 \, e^{-r^2/4Dt} \left[\frac{r^2+a^2-b^2}{2ar}\right] dr$$

$$= \frac{Dt}{a} \left\{ e^{-W_2} \left(u_2^2 + 4Dt - u_1u_2\right) - e^{-W_1} \left(u_1^2 + 4Dt - u_1u_2\right) \right\} . \qquad (5.4.6)$$

Similarly, the first integral in (5.4.4) can be expressed as:

$$- \int_{b-a}^{b+a} r^2 \, e^{-r^2/4Dt} \left[\frac{r^2+b^2-a^2}{2br}\right] dr$$
$$= \frac{Dt}{b} \left\{ e^{-W_2} \left(u_2^2 + 4Dt + u_1u_2\right) - e^{-W_1} \left(u_1^2 + 4Dt + u_1u_2\right) \right\} . \qquad (5.4.7)$$

Evaluating the second integral in (5.4.3), we have

$$\frac{1}{3} \int_{b-a}^{b+a} r^2 \, e^{-r^2/4Dt} \, \frac{(r^2+a^2-b^2)^3}{8a^3r^3} \, dr$$

$$= - \frac{Dt}{12a^3} \left\{ e^{-W_2} \left[u_2^4 + 8Dt \quad u_2^2 + 32D^2t^2 - 3u_1u_2^3 - 12u_1u_2Dt + 3u_1^2u_2^2\right] \right.$$

$$\left. - e^{-W_1}\left[u_1^4 + 8Dt \quad u_1^2 + 32D^2t^2 - 3u_1^3u_2 - 12u_1u_2Dt + 3u_1^2u_2^2\right] \right\}$$

$$- \frac{(u_1u_2)^3}{24a^3} \int_{u_1}^{u_2} \frac{1}{r} \, e^{-r^2/4Dt} \, dr. \qquad (5.4.8)$$

Similarly the second integral in (5.4.4) can be expressed as:

$$\frac{1}{3}\int_{b-a}^{b+a} r^2 \cdot e^{-r^2/4Dt}\,\frac{(r^2+b^2-a^2)^3}{8b^3r^3}\,dr$$

$$= -\frac{Dt}{12b^3}\left\{e^{-W_2}\left[u_2^4 + 8Dt\ \ u_2^2 + 32D^2t^2 + 3u_1u_2^3 + 12u_1u_2Dt + 3u_1^2u_2^2\right]\right.$$

$$\left. - e^{-W_1}\left[u_1^4 + 8Dt\ \ u_1^2 + 32D^2t^2 + 3u_1^3u_2 + 12u_1u_2Dt + 3u_1^2u_2^2\right]\right\}$$

$$+ \frac{(u_1u_2)^3}{24b^3}\int_{u_1}^{u_2}\frac{1}{r}\,e^{-r^2/4Dt}\,dr. \qquad (5.4.9)$$

Evaluating the third integral in (5.4.3) and (5.4.4), we have

$$\frac{2}{3}\int_{b-a}^{b+a} r^2\,e^{-r^2/4Dt} = -\frac{4}{3}\,Dt\left[u_2\,e^{-W_2} - u_1\,e^{-W_1} - \int_{u_1}^{u_2} e^{-r^2/4Dt}\,dr\right] \qquad (5.4.10)$$

Combining similar terms and upon simplification we have

$$I_2 + \left[\frac{b}{a}\right]^3 I_3 = \frac{8}{3}\,\frac{D^2t^2}{a^3}\,e^{-W_2}\,\{(a^2+b^2) - ab - 2\ Dt\}$$

$$- \frac{8}{3}\,\frac{Dt}{a^3}\,e^{-W_1}\,\{a^4 - a^3b + (a^2+b^2+ab)\ Dt - 2\ D^2t^2\}$$

$$+ \frac{4}{3}\,\frac{a^3+b^3}{a^3}\,Dt\sum_{k=0}^{\infty}\frac{(-1)^k\left[(a+b)^{2k+1} - (b-a)^{2k+1}\right]}{k!\ (2k+1)\ (4Dt)^k}\ . \qquad (5.4.11)$$

Putting (5.4.2), (5.4.11) into (5.4.5),

$$Q_{E,G}(t) = \frac{1}{\sqrt{\pi Dt}} \left\{ \left[-(b-a)\, e^{-W_1} + \sum_{k=0}^{\infty} \frac{(-1)^k (b-a)^{2k+1}}{k!\,(2k+1)\,(4Dt)^k} \right] \right.$$

$$+ \frac{Dt}{a^3} [(a^2+b^2)-ab-2\ Dt]\, e^{-W_2} - \frac{1}{a^3} [a^4-a^3b+(a^2+b^2+ab)\ Dt-2\ D^2t^2] e^{-W_1}$$

$$\left. + \frac{1}{2} \frac{a^3+b^3}{a^3} \sum_{k=0}^{\infty} \frac{(-1)^k [(a+b)^{2k+1} - (b-a)^{2k+1}]}{k!\,(2k+1)\,(4Dt)^k} \right\}$$

$$= \frac{1}{\sqrt{\pi Dt}} \left\{ \frac{Dt}{a^3} e^{-W_2} [(a^2+b^2)-ab-2\ Dt] - \frac{e^{-W_1}}{a^3} [(a^2+b^2+ab)\ Dt-2\ D^2t^2] \right.$$

$$+ \frac{1}{2} \left[1 + \frac{b^3}{a^3}\right] \sum_{k=0}^{\infty} \frac{(-1)^k (b+a)^{2k+1}}{k!\,(2k+1)\,(4Dt)^k}$$

$$\left. + \frac{1}{2} \left[1 - \frac{b^3}{a^3}\right] \sum_{k=0}^{\infty} \frac{(-1)^k (b-a)^{2k+1}}{k!\,(2k+1)\,(4Dt)^k} \right\}. \qquad (5.4.12)$$

When $E = G$, i.e. $b = a$, we have

$$Q_{E,G}(t) = \frac{1}{\sqrt{\pi Dt}} \left\{ \frac{Dt}{a^3} (a^2 - 2\ Dt)\, e^{-a^2/Dt} - \frac{1}{a^3} (3a^2\ Dt - 2\ D^2t^2) \right.$$

$$\left. + \sum_{k=0}^{\infty} \frac{(-1)^k (2a)^{2k+1}}{k!\,(2k+1)\,(4Dt)^k} \right\}. \qquad (5.4.13)$$

Expand and combine similar terms in (5.4.13), upon simplification, we have

$$Q_{E,G}(t) = \frac{3a^3}{Dt\sqrt{\pi Dt}} \sum_{k=0}^{\infty} \frac{(-1)^k\, a^{2k}}{(2k+3)(k+2)(k+3)(Dt)^k\, k!}$$

which is identical to eqn. (5.3.8).

APPENDIX I

DISTRIBUTION OF RELATIVE DISPLACEMENT

Let D_i, D_j be the diffusion coefficient of i–fold and j–fold disk respectively, both disks execute free Brownian motion in two dimensions. Under the assumption of independence of movements of each disk group, the distribution of relative displacement will be derived as follow.

At time 0, i–fold and j–fold disks are both at origin 0. After time t the position vector $\vec{r}_i = (x_i, y_i)$ for i–fold $\vec{r}_i = (x_j, y_j)$ for j–fold is normally distributed with the same vector $\vec{0}$ and covariance matrix Σ_i and Σ_j respectivedly.

That is, for i–fold disk, $\vec{r}_i = (x_i, y_i) \sim N(\vec{0}, \Sigma_i)$

where
$$\Sigma_i = \begin{bmatrix} 2D_i t & 0 \\ 0 & 2D_i t \end{bmatrix}$$

or the probability density function $P_t(\vec{r}_i)$ of $\vec{r}_i$ is

$$P_t(\vec{r}_i) = (2\pi)^{-1} |\Sigma_i|^{-\frac{1}{2}} \exp\left[-\frac{1}{2} (x_i, y_i)\, \Sigma_i^{-1} (x_i, y_i)'\right]$$

$$= (4\pi D_i t)^{-1} \exp\left[-\frac{1}{2} \frac{(x_i^2 + y_i^2)}{2D_i t}\right]$$

For j–fold disk,

$$\vec{r}_i = (x_j, y_j) \sim N(\vec{0}, \Sigma_j)$$

where

$$\Sigma_j = \begin{bmatrix} 2D_j t & 0 \\ 0 & 2D_j t \end{bmatrix}$$

and the probability density function $P_t(\vec{r}_j)$ of $\vec{r}_j$ is

$$P_t(\vec{r}_j) = (2\pi)^{-1}|\Sigma_i|^{-\frac{1}{2}} \exp\left[-\frac{1}{2}(x_j,y_j)\,\Sigma_j^{-1}(x_j,y_j)'\right]$$

$$= (4\pi D_j t)^{-1} \exp\left[-\frac{1}{2}\frac{(x_j^2 + y_j^2)}{2D_j t}\right].$$

Since $\vec{r}_i$, $\vec{r}_j$ are independent, using well known property is multivariate normal distribution (see Srivastava and Kharti (1979) page 46),

we have $$\vec{r}_i - \vec{r}_j = N(\vec{0}, \Sigma_i + \Sigma_j)$$

i.e. $$P_t(\vec{r}_1 - \vec{r}_2) = [4\pi(D_i+D_j)t]^{-1} \exp\left[-\frac{1}{2}\frac{(x_i-x_j)^2 + (y_i-y_j)^2}{2(D_i+D_j)t}\right].$$

On comparing this distribution of the relative displacements with the corresponding result for the individual displacements, we conclude that the relative displacements do follow the laws of Brownian motion with the diffusion coefficient $D_i + D_j$. In fact, it is also true for n dimensions.

APPENDIX II

CUBIC SPLINE INTERPOLATION METHOD

Given the data $g(t_1)$, ..., $g(t_n)$ with $a = x_1 <, ..., < x_n = b$, a piecewise cubic interpolant f to g can be constructed as follows. On each interval $[x_i, x_{i+1}]$, we have f agree with some polynomial P_i of order 4,

$$f(t) = P_i(t) \qquad \text{for} \qquad x_i \le t \le x_{i+1} \text{ for some } P_i \in \mathbb{P}_4 \; .$$

$$i = 1, ..., n-1$$

where $\mathbb{P}_4$ is the linear space of all polynomial of order 4. The i–th polynomial piece P_i is made to satisfy the conditions

$$P_i(x_i) = g(x_i),\ P_i(x_{i+1}) = g(x_{i+1})$$

and $$P_i(x_i) = s_i,\ P_i'(x_{i+1}) = s_{i+1}$$

for $$i = 1,2, ..., n-1.$$

Here s_1, ..., s_n are free parameters. The resulting piecewise function f agrees with g at x_1, ..., x_n and $f \in C'[a,b]$.

By Newton form and divided difference (see de Boor (1978), page 4) P_i, P_i can be expressed as

$$P_i(t) = C(i,0) + C(i,1)(t-x_i) + C(i,2)(t-x_i)^2 + C(i,3)(t-x_i)^3$$

where $$t \in [x_i, x_{i+1}]$$

with $$C(i,0) = P_i(x_i) = g(x_i)$$

$$C(i,1) = P_i'(x_i) = s_i$$

$$C(i,2) = \frac{P_i''(x_i)}{2}$$

and

$$C(i,3) = \frac{P_i'''(x_i)}{6}$$

C(i,1), C(i,2) and C(i,3) can be obtained by using ICSCCU in IMSL. The algorithm and details are discussed in Chapter IV of de Boor's book (page 49–59).

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