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# Exact solutions for diffusion–reaction processes in one dimension: II. Spatial distributions

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**Abstract.** As in an earlier paper, this paper examines one-dimensional diffusion-reaction processes. Exact results are given for one-dimensional polymerisation (cluster-cluster aggregation) occurring on subsets of $Z$, the infinite lattice, or $R$, the infinite line; the subsets may have periodic, absorbing or reflecting boundary conditions. The earlier paper gave spatially averaged polymer concentrations; this paper describes the spatial distribution of the concentrations. Our results have corollaries applying to coalescing random walks, and to binary and $n$-ary annihilation, since these are just polymerisation, modulos 1, 2 or $n$. Through well known dualities, our results also apply implicitly to the $T=0$ limit of the kinetic Ising model and to two interacting particle processes, the invasion and voter models.

## 1. Introduction

An earlier paper (Spouge 1988, hereafter referred to as I) considered a diffusion-reaction polymerisation process called 'Ppoly'. Ppoly is a one-dimensional irreversible cluster-cluster (CL-CL) aggregation process. CL-CL in higher dimensions provides a theoretical description of many aggregation phenomena, including galaxy formation from cosmic dust, aerosol coalescence, rainfall from clouds and even chemical polymerisation.

Scaling theory (de Gennes 1979), fractals (Family and Landau 1984) and the Smoluchowski coagulation equation (Drake 1972) provide models of aggregation, but make approximations of uncertain accuracy. Much theoretical effort has tried to estimate inaccuracies in these approximations, particularly when the approximations ignore spatial fluctuations (Kang and Redner 1984, 1985). Theories accounting for dimensionality can be tested by comparison to this paper since they should correctly predict one-dimensional behaviour.

This paper also discusses 'Pcoal', a process consisting of identical particles executing one-dimensional coalescing random walks, and 'Pnihil', a model for one-dimensional diffusion-limited binary annihilation, such as the thermal soliton-antisoliton interactions occurring after the photoexcitation of trans-polyacetylene (Răcz 1985). Like Ppoly, Pcoal and Pnihil also allow testing of theoretical approximations. Kang and Redner (1984) have done Monte Carlo simulations of all three processes, which we now define.

Ppoly takes place on a 'medium', a subset of $Z$ (the lattice of integers) or $R$ (the real line). $Z$ and $R$ are the only media examined in the main body of this paper. We defer until later the complications introduced by periodic, absorbing or reflecting boundaries; these will be handled by the principle of reflection.

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Ppoly begins at time $t_0 = 0$ by distributing, possibly at random, a set of points on the medium. Polymer chemistry provides a convenient terminology: we call the initial points 'monomers'. After $t_0$, all monomers diffuse identically and independently and aggregate irreversibly when they meet. The resulting point aggregates ('polymers') are indistinguishable from monomers in their diffusive behaviour and also continue to aggregate when they meet.

A polymer containing $k$ monomers is a '$k$-mer'. Because it is useful to think of a $k$-mer as containing $k$ monomers, and to think of each of these monomers as retaining a unique history, we distinguish between the 1-mers present at $t_0$ ('monomers'), and those present at later times ('1-mers'). We will also use $t_0$ instead of 0, particularly as a functional argument, to distinguish between the temporal and spatial zeros.

$c_k(x, t)\,\mathrm{d}x$ is defined to be the probability at time $t$ of finding a $k$-mer in the interval $[x, x+\mathrm{d}x)$, in the limit as $\mathrm{d}x \to 0$. This probability includes the effect of the initial distribution of monomer positions and all realisations of diffusive processes. For brevity, we shall say that $c_k(x, t)$ is the concentration of $k$-mers *at position* $x$. In the following, this 'position convention', the use of a phrase like 'at position $x$', always implies an implicit limit like $\mathrm{d}x \to 0$.

In order to achieve a unity of exposition, the position convention will apply to both $Z$ and $R$. On $R$, $c_k(x, t)$ is not always a generalised function (Lighthill 1978); on $Z$, by necessity, it always is. As an example, three 'special' initial monomer distributions play an important role in this paper: (a) the Poisson distribution on $R$, giving a uniform initial monomer distribution (for convenience, we scale length so that, on the average, this distribution places one monomer in each unit interval); (b) the delta distribution on $Z$ or $R$, which places with certainty a monomer at each point of $Z$; and (c) the half-delta distribution on $Z$ or $R$, which places, independently with probability $\frac{1}{2}$, a monomer at each point of $Z$. The special initial distributions give the following monomer concentrations:

$$c_1(x, t_0) = 1 \tag{1.1}$$

$$c_1(x, t_0) = \sum_{k=-\infty}^{\infty} \delta(x-k) \tag{1.2}$$

$$c_1(x, t_0) = \sum_{k=-\infty}^{\infty} \tfrac{1}{2}\delta(x-k). \tag{1.3}$$

$\delta(y)$ is the Dirac delta, defined by $\int f(y)\delta(y)\,\mathrm{d}y = f(0)$ for any ordinary function $f$ (Lighthill 1978, p 17). In passing, note that (1.1) and (1.3) do not describe the Poisson and half-delta distributions completely, since these distributions place every monomer *independently of the placement of any other monomer.*

The total concentration of polymers at position $x$ at time $t$ is

$$c_+(x, t) = \sum_{k=1}^{\infty} c_k(x, t). \tag{1.4}$$

This is also the concentration of 1-mers in the coalescence process (Kang and Redner 1984), Pcoal, in which two 1-mers coalesce to form another 1-mer: 1-mer + 1-mer → 1-mer. Pcoal is essentially Ppoly (mod 1). Because its 1-mers are executing coalescing random walks, Pcoal on $Z$ is the process dual to the Clifford-Sudbury voter model (1973), a type of interacting-particle system (Liggett 1985).

The binary annihilation process (Kang and Redner 1984, Torney and McConnell 1983, Lushnikov 1987, Balding 1988), Pnihil, is essentially Ppoly (mod 2). The following reactions are possible: 1-mer + 1-mer → 0-mer, 0-mer + 1-mer → 1-mer and 0-mer + 0-mer → 0-mer. One usually considers the 0-mers to be non-existent, and monomers to annihilate one another when they meet. Because its 1-mers are executing annihilating random walks, Pnihil on $Z$ is related to the $T = 0$ limit of the Ising model (Glauber 1963, Răcz 1985). The concentrations of 1-mers in both Pnihil and Ppoly (mod 2) are

$$c_{-}(x, t) = \sum_{k=1}^{\infty} c_{2k-1}(x, t). \tag{1.5}$$

Generalising (1.5) yields the concentrations in the $n$-ary annihilation process, Ppoly (mod $n$), in which a polymer is annihilated by the $n$th monomer to join it. Results for Ppoly therefore have implications for the coalescence, binary and $n$-ary annihilation processes.

For brevity in the following, unsubscripted $c$ will indicate statements or equations which hold if the $c$ are subscripted by '$k$', '+' or '−'. As an illustration, I focused on $c_k(t)$, the number of $k$-mers per unit length *averaged over the medium in question.* In this paper, in order to account for spatial distributions, the focus is on $c_k(x, t)$, the concentration of $k$-mers *at position* $x$. Spatially averaged analogues such as $c_k(t)$ may be identified by the omission of a spatial argument (cf $c_k(x, t)$) and are defined on $Z$ or $R$ by

$$c(t) \triangleq \lim_{P \to \infty} (1/2P) \int_{[-P,P)} c(x, t)\, \mathrm{d}x \tag{1.6}$$

when the limit on the right exists. ($\triangleq$ indicates a definition.) The interval notation for ranges of integration will be convenient in this paper.

The omission of the subscript '$k$' in (1.6) indicates that $c_{+}(t)$ and $c_{-}(t)$ can be defined analogously. Equation (1.6) gives $c_k(t)$ a precise physical interpretation: it is the *expectation* at time $t$ of the number of $k$-mers per unit length averaged over the medium in question. The expectation, like the one implicit in the definition of $c_k(x, t)$, is taken over all initial monomer positions and over all realisations of the diffusive processes for Ppoly. By contrast to $c_k(x, t)$, the concentration of $k$-mers *at position* $x$, this paper simply refers to $c_k(t)$ as 'the concentration of $k$-mers'.

Our three special distributions are all invariant under translation through $L = 1$. In order to examine spatial variations, we perturb the initial distributions of (1.1)–(1.3) by adding or removing a single monomer. These perturbations propagate through time as $\Delta c(x, t)$, a 'perturbation at position $x$' to $c(x, t)$, the concentration at position $x$. Because of the averaging over the entire medium, however, a single monomer perturbation has no effect on the concentrations $c(t)$. In order to follow the perturbation to the entire medium, we define

$$\Delta c(M, t) \triangleq \int \Delta c(x, t)\, \mathrm{d}x \tag{1.7}$$

where '$M$' will be replaced by '$R$' or '$Z$', whichever is the relevant medium. Unspecified ranges of integration like the one above are assumed to be over the entire medium. By contrast to $\Delta c(x, t)$, the perturbation *at position* $x$, we simply refer to $\Delta c(M, t)$ as a 'perturbation'.

If $c_1^0(x, t)$ is the relevant initial monomer distribution from (1.1)–(1.3) and $\Delta c_1(x, t)$ is its perturbation, the perturbations of the special distributions $c_1(x, t) =$

$c_1^0(x, t)+\Delta c_1(x, t)$ examined in this paper are

$$c_1(x, t_0)=1+\delta(x) \tag{1.8}$$

$$c_1(x, t_0)=\sum_{k=-\infty}^{\infty} \delta(x-k)-\delta(x) \tag{1.9}$$

$$c_1(x, t_0)=\sum_{k=-\infty}^{\infty} \tfrac{1}{2}\delta(x-k)-\tfrac{1}{2}\delta(x). \tag{1.10}$$

The perturbed special distributions are: (a) the Poisson distribution with a monomer at position 0 added; (b) the delta distribution with the monomer at position 0 removed; and (c) the half-delta distribution with the monomer at position 0, if it exists, removed (the choice of adding or removing the monomer in case (c) was arbitrary).

Armed with these preliminaries, we now explore the spatial distributions occurring in Ppoly, Pcoal and Pnihil.

## 2. General results for concentrations and perturbations

We solve Ppoly by focusing on its most elementary events, the collisions of monomer pairs. The key idea allowing a solution is that, in one dimension, the monomers are linearly ordered. This fact forces any polymer containing two given monomers to contain every monomer that started between them. The $k$-mer concentrations at position $x$ are therefore related to certain events involving the collision of monomer pairs.

Let us begin by noting that each polymer has two directions in which to meet other polymers. Let us call the positive direction, 'right', and the negative, 'left'. Within each polymer, it will be convenient to define a 'leftmost' monomer, the one with the leftmost (i.e. most negative) initial position.

$c_k(x, t)$ is the probability at time $t$ of finding a $k$-mer at position $x$. (Recall the 'position convention': 'at position $x$' implies an implicit limit.) Exactly one of the $k$ monomers in a $k$-mer is the leftmost monomer. Hence $c_k(x, t)$ is also the sum over all monomers, $P_0$, of the probability that, at time $t$, $P_0$ is the leftmost monomer in a $k$-mer at position $x$. This probability can be calculated as follows.

Let $P_{-1}, P_0, \ldots, P_{k-1}, P_k$ be consecutive monomers, ordered in the positive direction at $t_0$, but otherwise arbitrary. For the time being, let us consider a single initial state so that the initial positions of these monomers are fixed. Let $A_0$ be the event that, at time $t$, (a) the two monomers $P_0$ and $P_{k-1}$ are in the same polymer and (b) the polymer is at position $x$. Let $A_1$ be the same event as $A_0$, but for $P_{-1}$ and $P_{k-1}$ instead of $P_0$ and $P_{k-1}$; $A_2$, for $P_{-1}$ and $P_k$; and $A_3$, for $P_0$ and $P_k$. $A_0 \sim (A_1 \cup A_3)$ is the event that, at time $t$, $P_0$ is the leftmost monomer in a $k$-mer at position $x$ containing $P_0, P_1, \ldots, P_{k-1}$.

$A_1 \subset A_0$, because the linear ordering of the monomers in one dimension implies that a polymer containing both $P_{-1}$ and $P_{k-1}$ must also contain $P_0$. Also, $A_3 \subset A_0$ and $A_1 \cap A_3 = A_2$. A Venn diagram of the $A$ shows that

$$P(A_0 \sim (A_1 \cup A_3))=\sum_{k=0}^{3}(-1)^k P(A_k). \tag{2.1}$$

Summing (2.1) over all possible initial positions for the monomer pairs $(P_0, P_{k-1})$, $(P_{-1}, P_{k-1})$, $(P_0, P_k)$ and $(P_{-1}, P_k)$ gives the probability defining $c_k(x, t)$. The summation requires: (a) the distribution of the initial positions $y$ and $z$ for the given monomer pairs; and (b) the probability that, at time $t$, two monomers starting at given positions $y$ and $z$ have met and the polymer containing them is at position $x$.

In order to account for the initial monomer positions, let $\beta_k(y, z)\,\mathrm{d}y\,\mathrm{d}z$ be the probability that there is some monomer, say $P_0$, in the interval $[y, y+\mathrm{d}y)$ and that $P_k$, the corresponding $k$th neighbour, is in the interval $[z, z+\mathrm{d}z)$, as $\mathrm{d}y, \mathrm{d}z \to 0$. We define $\beta_k(y, z) \triangleq 0$ when $z<y$.

In order to account for monomer collisions and the position of the resultant polymer, define the annihilation Green function $a(x, t; y, z)$ to be the probability that, at time $t$, (a) two monomers $P_0$ and $P$ starting at positions $y$ and $z$ are in the same polymer; and (b) the polymer is at position $x$. Because $\beta_k(y, z) \triangleq 0$ when $z<y$, the value of $a(x, t; y, z)$ for $z<y$ is irrelevant. (This is the case on $Z$ and $R$; for media with boundary conditions, we shall later extend the definition of $a(x, t; y, z)$ to the regime $z<y$.)

If $\Sigma$ denotes a summation over all monomers $P_0$, double-integrating over the possible initial positions of the monomer pairs gives

$$\begin{aligned}
\sum P(A_0) &= \int\int a(x, t; y, z)\beta_{k-1}(y, z)\,\mathrm{d}y\,\mathrm{d}z \\
\sum P(A_1) = \sum P(A_3) &= \int\int a(x, t; y, z)\beta_k(y, z)\,\mathrm{d}y\,\mathrm{d}z \qquad (2.2)\\
\sum P(A_2) &= \int\int a(x, t; y, z)\beta_{k+1}(y, z)\,\mathrm{d}y\,\mathrm{d}z.
\end{aligned}$$

For an isolated diffusing particle, let $\gamma(x-y, t)$ be the probability that the particle diffuses from position $y$ to position $x$ in the time interval $[0, t]$. Recall that $c_1(y, t_0)$ is the probability at time $t_0$ of finding a monomer at position $y$. When $k=1$, the physical interpretation of $A_0$ preceding (2.1) demands that $\Sigma P(A_0) = \int \gamma(x-y, t)\, c_1(y, t_0)\,\mathrm{d}y$. The following definitions therefore make the physical interpretation consistent with (2.2): $a(x, t; y, y) \triangleq \gamma(x-y, t)$ and $\beta_0(y, z) \triangleq c_1(y, t_0)\delta(z-y)$.

In all cases, then, (2.1) and (2.2) now give

$$\begin{aligned}
c_k(x, t) &= \int\int a(x, t; y, z)[\beta_{k-1}(y, z) - 2\beta_k(y, z) + \beta_{k+1}(y, z)]\,\mathrm{d}y\,\mathrm{d}z \\
&\triangleq \int\int a(x, t; y, z) b_k(y, z)\,\mathrm{d}y\,\mathrm{d}z. \qquad (2.3)
\end{aligned}$$

If '+' or '−' replaces '$k$' in the first and last expressions of (2.3), equations (1.4) and (1.5) define analogous kernels $b_+(y, z)$ and $b_-(y, z)$ for $c_+(x, t)$ and $c_-(x, t)$:

$$b_+(y, z) \triangleq \beta_0(y, z) - \beta_1(y, z) \qquad (2.4)$$

$$b_-(y, z) \triangleq \beta_0(y, z) + 2\sum_{k=1}^{\infty} (-1)^k \beta_k(y, z). \qquad (2.5)$$

Substituting (2.4) back into the analogue of (2.3) explains the simplicity of (2.4): the total polymer concentration at position $x$ is equal to the concentration of those monomers at position $x$ which have not met their right-hand neighbour. The sum in (2.5) also has a simple interpretation: it is the difference between the probability densities for a monomer at position $y$ having an even and an odd neighbour at position $z$.

The next section gives $\beta_k(y, z)$ for the special distributions. With those $\beta_k(y, z)$ in hand, the annihilation Green function $a(x, t; y, z)$ completely determines the polymer concentrations. We shall now relate $a(x, t; y, z)$ to $\gamma(x-y, t)$, the probability that an isolated diffusing particle moves from position $y$ to position $x$ in the time interval $[0, t]$.

For future reference, on $Z$, a continuous-time symmetric nearest-neighbour random walk (Feller 1971, p 59) with diffusion constant $D=1$ gives

$$\gamma(x, t)=\exp(-2t)I_x(2t)\sum_{k=-\infty}^{\infty}\delta(x-k). \tag{2.6}$$

$I_x$ is a modified Bessel function (Abramowitz and Stegun 1972, p 374). Note the use of the generalised functions in (2.6): the infinite row of delta functions places an atom of size $\exp(-2t)I_k(2t)$ on the points $k$ of $Z$.

On $R$, driftless Brownian motion (Krank 1979, p 12) with diffusion constant $D=1$ gives

$$\gamma(x, t)=(4\pi t)^{-1/2}\exp(-x^2/4t). \tag{2.7}$$

Since the unit of time can always be normalised to make $D=1$, equations (2.6) and (2.7) involve no loss of generality.

We will show that on both $Z$ and $R$

$$a(x, t; y, z)=\gamma(x-y, t)\int_{(-\infty,x]}\gamma(w-z, t)\,\mathrm{d}w+\gamma(x-z, t)\int_{(x,\infty)}\gamma(w-y, t)\,\mathrm{d}w. \tag{2.8}$$

In actual calculations for $Z$, the integrals are replaced by sums. We have, however, unified the presentation by using generalised functions (see, e.g., equation (2.6)). This causes no difficulty (Lighthill 1978, p 25), except when integrals like $\int_{(-\infty,x]}\delta(w-x)\,\mathrm{d}w$ necessitate an 'endpoint convention' for $Z$: $\int_{(-\infty,x]}\delta(w-x)\,\mathrm{d}w\triangleq 1$ and $\int_{(x,\infty)}\delta(w-x)\,\mathrm{d}w\triangleq 0$. The endpoint convention can be verified by rewriting the integrals in (2.8) as sums.

Equation (2.8) can be proved by the principle of reflection (see figure 1). Consider a single point $(Y, Z)$ diffusing in two dimensions, where the coordinates of the point start at $(y, z)$, within the shaded area of figure 1 where $y<z$, and always equal the one-dimensional positions of two diffusing polymers, which we call the $y$- and $z$-polymers. If the point hits the line $Y=Z$, the $y$- and $z$-polymers have met, but we continue to follow the diffusion of the point, regarding $Z$ as the position of the resulting larger polymer. Let the point be at position $(w, x)$ at time $t$. If $w>x$ (the black point $(w, x)$ in the unshaded area), the two-dimensional diffusion crossed the line $Y=Z$. Otherwise, if $w\leqslant x$ (the white point $(w, x)$ in the shaded area), then every path from $(y, z)$ to $(w, x)$ meeting the line $Y=Z$, when reflected across $Y=Z$ after the path's first intersection with $Y=Z$, corresponds to exactly one path from $(y, z)$ to $(x, w)$. Integrating the probabilities over two half-lines starting from $(x, x)$, one going horizontally to the right, the other going vertically down, gives (2.8).

The following intermediate result is helpful: let $b(y, z)$ be any of $b_k(y, z)$, $b_+(y, z)$ or $b_-(y, z)$ and let $c(x, t)$ be the integral resulting from substituting $b(y, z)$ into the analogue of (2.3). Standard manipulation of the multiple integrals resulting from (2.3) yields

$$c(x, t)=\int\int\int_{w\in[z,\infty)}\gamma(w, t)\gamma(y, t)b(y+x, z+x)\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}w$$

$$+\int\int\int_{w\in(-\infty,z)}\gamma(w, t)\gamma(z, t)b(y+x, z+x)\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}w. \tag{2.9}$$

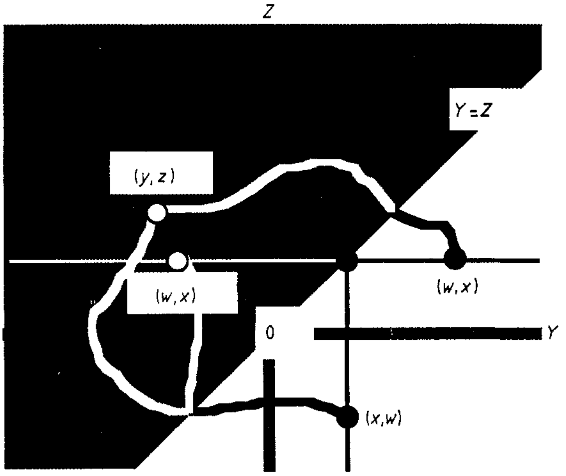

**Figure 1.** Two diffusing monomers start at positions $y$ and $z$. They meet and the polymer containing them then ends at position $x$. This process is equivalent to a two-dimensional diffusion starting at the point $(y, z)$, intersecting the line $Y=Z$ and, augmented thereafter by a dummy diffusing $Y$ coordinate, diffusing to the line $Z=x$. By necessity, every two-dimensional diffusion ending on the black half-line $Z=x$ intersects the line $Y=Z$; diffusions intersecting the line $Y=Z$ and ending on the white half-line $Z=x$ can be reflected across $Y=Z$ at their first intersection with $Y=Z$ to end on the indicated black half-line of $Y=x$.

We now give a derivation of known results for $c(t)$ from the results for $c(x, t)$. The derivation may help to unify presentations of one-dimensional diffusion-reaction processes, but it does involve manipulating multiple integrals containing generalised functions. Because a convenient reference justifying these manipulations does not exist, we can only outline plausibility arguments for them. The derivation probably carries through for any 'physical' initial distribution, since I have verified independently its results for our special initial distributions.

An earlier paper (Spouge 1988) presented spatially averaged results on $Z$ or $R$ in terms of the following quantities:

$$\begin{aligned} c_0 &\triangleq \lim_{P\to\infty} (1/2P) \int_{[-P,P)} c_1(y, t_0)\,\mathrm{d}y \\ b(u) &\triangleq \lim_{P\to\infty} (1/2P) \int_{[-P,P)} b(y, y+u)\,\mathrm{d}y \qquad (2.10) \\ a(t; u) &\triangleq \int a(v, t; 0, u)\,\mathrm{d}v. \end{aligned}$$

Replacing $b(u)$ in (2.10) by $c_0\, b(u)$ gives the notation used in I. This paper changed the notation in order to increase the resemblance between equations involving concentrations and those involving perturbations. Paper I gives $\beta_k(u)$ for the three special distributions of this paper. Multiplying $\beta_k(u)$ from I by $c_0$ gives $\beta_k(u)$ in the present notation.

Interpretations for $c_0$, $b(u)$ and $a(t; u)$ follow. $c_0$ is the initial concentration of monomers, averaged over the medium. $b(u)c_0^{-1}$ is esentially $b(y, z)$, but for a randomly chosen monomer. For example, $\beta_k(y, z)$ is the probability of finding an initial monomer at position $y$ and its $k$th neighbour at position $z$; $\beta_k(u)c_0^{-1}$ is the probability that a randomly chosen monomer has its $k$th neighbour at a distance $u$ to the right. Equations (2.3)-(2.5) suggest the relationships between $b_k(u)$, $b_+(u)$, $b_-(u)$ and $\beta_k(u)$: these are given in I.

The diffusions of equations (2.6) and (2.7) are spatially homogeneous, implying that $a(y+v, t; y, y+u) = a(v, t; 0, u)$. When $a(y+v, t; y, y+u) = a(v, t; 0, u)$, $a(t; u)$ is the probability that two monomers starting at 0 and $u$ (or at $y$ and $y+u$) are in the same polymer by time $t$. Like the values of $a(x, t; y, z)$ for $z<y$, because $\beta_k(u)=0$ when $u<0$, the values $a(t; u)$ for $u<0$ are irrelevant.

$\gamma(-x, t) = \gamma(x, t)$ (the diffusions are symmetric) and $\int \gamma(x, t)\gamma(w-x, t)\,\mathrm{d}x = \gamma(w, 2t)$ (a point diffusing to position $w$ in the time interval $[0, 2t]$ diffused to some position $x$ in the time interval $[0, t]$, and then diffused a distance $w-x$ in the remaining time interval $[t, 2t]$). Hence substituting (2.8) into (2.10) yields

$$a(t; u) = \int_{[u,\infty)} \gamma(w, 2t)\,\mathrm{d}w + \int_{(u,\infty)} \gamma(w, 2t)\,\mathrm{d}w. \tag{2.11}$$

Equation (2.11) shows that $a(t; 0) = 1$. With the endpoint convention on $Z$, (2.11) agrees with results from I. On $R$ open endpoints produce the same results as closed ones. This leads immediately to a useful relationship on $R$:

$$(\mathrm{d}/\mathrm{d}u)a(t; u) = -2\gamma(u, 2t). \tag{2.12}$$

On $Z$ or $R$, when the diffusions have diffusion constant $D=1$, $a(x, t; y, z) = \mathrm{O}\{\exp[-(x-y)^2/4t]\}\,\mathrm{O}\{\exp[-(x-z)^2/4t]\}$ as $|x-y|$, $|x-z| \to \infty$. This rapid decay is important because, for any fixed time $t$ and sufficiently large $P$, 'almost all' monomers starting at position $y$ give rise to polymers at positions $x$ within $[y-\sqrt{P}, y+\sqrt{P})$. (The choice of $f(P) = \sqrt{P}$ is arbitrary; in the following, $f(P)$ need only satisfy $\lim_{P\to\infty} f(P) = \infty$ and $\lim_{P\to\infty} P^{-1} f(P) = 0$.) This implies that 'almost all' polymers at positions $x$ within $[-P, P)$ originate from monomers starting at positions $y$ or $z$ within $[-P-\sqrt{P}, P+\sqrt{P})$. A related property holds for 'physical' initial monomer distributions: at any fixed time $t$, as $P\to\infty$, $\mathrm{O}(P)$ polymers within $[-P-\sqrt{P}, P+\sqrt{P})$ contain monomers originating from within $[-P-\sqrt{P}, -P)$ or $[P, P+\sqrt{P})$. These facts justify the necessary truncations, the change of variable from $x$, $y$ and $z$ to $v \triangleq x-y$, $y$ and $u \triangleq z-y$, and the interchanges in the order of limits and integration in the following:

$$\begin{aligned}
&\lim_{P\to\infty} (1/2P) \int_{[-P,P)} \int\int a(x, t; y, z) b(y, z)\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}x \\
&\quad = \lim_{P\to\infty} (1/2P) \int\int_{[-P-\sqrt{P},P+\sqrt{P})} \left(\int_{[-\sqrt{P},\sqrt{P})} a(y+v, t; y, y+u)\,\mathrm{d}v\right) \\
&\quad\quad \times b(y, y+u)\,\mathrm{d}y\,\mathrm{d}u \\
&\quad = \lim_{P\to\infty} (1/2P) \int\int_{[-P-\sqrt{P},P+\sqrt{P})} a(t; u) b(y, y+u)\,\mathrm{d}y\,\mathrm{d}u.
\end{aligned} \tag{2.13}$$

Equations (1.6) and (2.13), and then equation (2.10), yield

$$c(t)=\lim_{P\to\infty}(1/2P)\int_{[-P,P)}\int\int a(x,t;y,z)b(y,z)\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}x$$
$$=\int a(t;u)b(u)\,\mathrm{d}u. \tag{2.14}$$

Equation (2.14) is the basic equation in I, derived there by other means.

For a probabilistic distribution of monomer positions which is invariant under translation through a (not necessarily minimal) period $L$, e.g. the special distributions of this paper, spatial averages in (2.15) may be taken over a single period:

$$c(t)=L^{-1}\int_{[0,L)}c(x,t)\,\mathrm{d}x. \tag{2.15}$$

Because $c(x,t)$ is a linear functional of $\beta_k(y,z)$ (note that it is *not* a linear functional of the initial monomer concentrations $c_1(x,t_0)$), $\Delta c(x,t)$ and $\Delta b(y,z)$, the perturbations of $c(x,t)$ and $b(y,z)$, are also related by (2.3). We therefore adopt standard perturbation notation: $c(x,t)=c^0(x,t)+\Delta c(x,t)$ and $b(y,z)=b^0(y,z)+\Delta b(y,z)$. For any perturbation $\Delta c_1(x,t_0)$ of the initial monomer distribution that decays rapidly as $|x|\to\infty$, e.g. a single monomer perturbation, a derivation similar to that for (2.14) but omitting averaging over $[-P,P)$ gives an expression for the perturbation to a medium:

$$\begin{aligned}\Delta b(u)&\triangleq\int\Delta b(y,y+u)\,\mathrm{d}y\\ \Delta c(M,t)&=\int a(t;u)\Delta b(u)\,\mathrm{d}u\end{aligned} \tag{2.16}$$

where, in specific cases, '$M$' is replaced by the relevant medium, $R$ or $Z$. We can now derive some results for the special distributions.

## 3. Results for the special initial distributions and their perturbations

Where possible, we shall now derive closed results for the Poisson, delta and half-delta initial distributions. Analytic expressions for the concentrations resulting from the unperturbed initial distributions are known (Torney and McConnel 1983, Lushnikov 1987, Balding 1988, Balding *et al* 1988, Spouge 1988) but this section gives both extra intermediate results and some perturbation results as well.

### 3.1. *The Poisson distribution*

Let $H(y)$ be the Heaviside unit function: $H(y)=0$ for $y<0$ and $H(y)=1$ for $y\geqslant 0$. For the Poisson distribution and $k\geqslant 1$

$$\begin{aligned}\beta_k^0(y,z)&=\exp[-(z-y)]\frac{(z-y)^{k-1}}{(k-1)!}H(z-y)\\ b_+^0(y,z)&=\delta(y-z)-\exp[-(z-y)]H(z-y)\\ b_-^0(y,z)&=\delta(y-z)-2\exp[-2(z-y)]H(z-y).\end{aligned} \tag{3.1}$$

Inserting $\lambda$ for 2 in the last two equations (3.1) allows 'parallel processing' of (2.9): the resulting multiple integrals not involving delta functions can be calculated by rotating the $w-y$ coordinate system for the first integral in (2.9) by $\pi/4$, integrating, and doubling the result. This gives

$$\begin{aligned} c_+^0(x,t) &= \exp(2t)\operatorname{erfc}(2t)^{1/2} \\ c_-^0(x,t) &= \exp(8t)\operatorname{erfc}(8t)^{1/2} \end{aligned} \tag{3.2}$$

where $\operatorname{erfc}(z) = (2/\sqrt{\pi})\int_z^\infty \exp(-z^2)\,\mathrm{d}z = 1-\operatorname{erf}(z)$ is the complementary error function (Abramowitz and Stegun 1972, p 297). Equation (2.15) with, e.g., $L=1$ shows that $c(t) = c^0(x,t)$ for this distribution.

Let $t_k(x) \triangleq x^{k-1}/(k-1)!$. When the Poisson distribution is perturbed by a monomer inserted at position 0, for $k \geqslant 1$

$$\begin{aligned} \Delta\beta_k(y,z) &= \exp[-(z-y)]\{\delta(y)t_k(z)H(z) + \delta(z)t_k(-y)H(-y) \\ &\qquad + [t_{k-1}(z-y) - t_k(z-y)]H(-y)H(z)\} \\ \Delta b_+(y,z) &= [\delta(y) - \mathrm{e}^{y}H(-y)][\delta(z) - \mathrm{e}^{-z}H(z)] \\ \Delta b_-(y,z) &= [\delta(y) - 2\,\mathrm{e}^{2y}H(-y)][\delta(z) - 2\,\mathrm{e}^{-2z}H(z)]. \end{aligned} \tag{3.3}$$

The first equation in (3.3) has three terms corresponding to: (a) at position $z>0$, the $k$th monomer to the right of the monomer at position 0; (b) at position $y<0$, the $k$th monomer to the left of the monomer at position 0; and (c) at position $z>0$, the $(k-1)$th monomer to the right of a monomer at position $y<0$ becoming the $k$th because of the inserted monomer at position 0.

Inserting $\lambda$ for 2 in the last two equations (3.3) allows 'parallel processing' of (2.16) to give

$$\Delta b(u) = \delta(u) - 2\lambda\,\mathrm{e}^{-\lambda u}H(u) + \lambda^2 u\,\mathrm{e}^{-\lambda u}H(u). \tag{3.4}$$

Substituting this into (2.16) and then using (2.12) to integrate by parts yields

$$\Delta c(R,t) = 2\int \gamma(u,2t)[(\mathrm{e}^{-\lambda u} - \lambda u\,\mathrm{e}^{-\lambda u})H(u)]\,\mathrm{d}u. \tag{3.5}$$

The first term of this integral is like the integrals relevant to (3.2). The second term is then derived by differentiating the first term with respect to the parameter $\lambda$. Substituting $\lambda=1$ and $\lambda=2$ gives

$$\begin{aligned} \Delta c_+(R,t) &= \exp(2t)\operatorname{erfc}(2t)^{1/2}(1-4t) + (2/\sqrt{\pi})(2t)^{1/2} \\ \Delta c_-(R,t) &= \exp(8t)\operatorname{erfc}(8t)^{1/2}(1-16t) + (4/\sqrt{\pi})(2t)^{1/2}. \end{aligned} \tag{3.6}$$

### 3.2. *The delta and half-delta distributions*

The following intermediate result from (2.9) is useful: on both $Z$ and $R$, when

$b(y,z) = \delta(y-j)\delta(z-k)$

$$c(x,t) = \gamma(j-x,t)\int_{[k-x,\infty)} \gamma(w,t)\,\mathrm{d}w + \gamma(k-x,t)\int_{(-\infty,j-x)} \gamma(w,t)\,\mathrm{d}w. \tag{3.7}$$

On $Z$, the above integrations are equivalent to striking out the delta functions in (2.6) for $\gamma(x, t)$ and replacing the integrals above by sums. The Bessel function identities (Feller 1971, p 60)

$$\begin{aligned}
&\exp[\tfrac{1}{2}(u+u^{-1})x] = \sum_{w=-\infty}^{\infty} u^{w} I_{w}(x) \\
&I_{-k}(x) = I_k(x) \qquad \text{for integral } k \qquad (3.8) \\
&I_k(x+y) = \sum_{w=-\infty}^{\infty} I_w(x) I_{k+w}(y)
\end{aligned}$$

will be useful

For the delta distribution on $Z$ or $R$,

$$\begin{aligned}
&\beta_k^0(y, z) = \sum_{j=-\infty}^{\infty} \delta(y-j)\delta(z-j-k) \\
&b_+^0(y, z) = \sum_{j=-\infty}^{\infty} \delta(y-j)[\delta(z-j)-\delta(z-j-1)] \qquad (3.9) \\
&b_-^0(y, z) = \sum_{j=-\infty}^{\infty} \delta(y-j)\left(\delta(z-j)+2\sum_{k=1}^{\infty}(-1)^k\delta(z-j-k)\right).
\end{aligned}$$

In conjunction with (3.7), these equations yield

$$\begin{aligned}
c_k^0(x, t) = &\sum_{j=-\infty}^{\infty} \gamma(j-x, t) \\
&\times\left[\left(\int_{[k-1,k)} - \int_{[k,k+1)} + \int_{[-k,-k+1)} - \int_{[-k-1,-k)}\right)\gamma(j-x+w, t)\,\mathrm{d}w\right] \\
c_+^0(x, t) = &\sum_{j=-\infty}^{\infty} \gamma(j-x, t)\int_{[-1,1)} \gamma(j-x+w, t)\,\mathrm{d}w \qquad (3.10) \\
c_-^0(x, t) = &\sum_{j=-\infty}^{\infty} \gamma(j-x, t)\sum_{k=0}^{\infty}(-1)^k\left[\left(\int_{[k,k+1)} + \int_{[-k-1,-k)}\right)\gamma(j-x+w, t)\,\mathrm{d}w\right].
\end{aligned}$$

On $Z$, (2.6) and (3.10) give

$$\begin{aligned}
&c_k^0(x, t) = \exp(-4t)[I_{k-1}(4t) - I_{k+1}(4t)] \sum_{j=-\infty}^{\infty} \delta(x-j) \\
&c_+^0(x, t) = \exp(-4t)[I_0(4t) + I_1(4t)] \sum_{j=-\infty}^{\infty} \delta(x-j) \qquad (3.11) \\
&c_-^0(x, t) = \exp(-4t) I_0(4t) \sum_{j=-\infty}^{\infty} \delta(x-j).
\end{aligned}$$

The row of delta functions places equally sized atoms at each point of $Z$. Equation (2.15) with $L=1$ shows that $c(t)\Sigma_{-\infty}^{\infty}\,\delta(x-j) = c(x, t)$ for the delta distribution on $Z$.

On $R$, (2.15) with $L=1$, when applied to (3.10), yields

$$\begin{aligned} c_k(t) &= \left(\int_{[k-1,k)} - \int_{[k,k+1)} + \int_{[-k,-k+1)} - \int_{[-k-1,-k)}\right)\int_{-\infty}^{\infty} \gamma(-x,t)\gamma(-x+w,t)\,\mathrm{d}x\,\mathrm{d}w \\ &= \left(\int_{[k-1,k)} - \int_{[k,k+1)} + \int_{[-k,-k+1)} - \int_{[-k-1,-k)}\right)\gamma(w,2t)\,\mathrm{d}w \qquad (3.12) \\ &= -\mathrm{erf}[(k-1)/(8t)^{1/2}] + 2\,\mathrm{erf}[k/(8t)^{1/2}] - \mathrm{erf}[(k+1)/(8t)^{1/2}] \\ c_+(t) &= \mathrm{erf}[(8t)^{-1/2}]. \end{aligned}$$

Figure 2($a$) plots $c_k(t)$ against $t$ for the unperturbed delta distribution on $R$. Figure 2($b$) plots $c_+(t)$ and $c_-(t)$ against $t$ for the same distribution on $Z$.

When the delta distribution is perturbed by deleting the monomer at position 0, for $k \geq 0$,

$$\begin{aligned} \Delta\beta_k(y,z) &= \sum_{j=-k}^{0} \delta(y-j)[\delta(z-j-k-1)-\delta(z-j-k)] - \delta(y)\delta(z-k-1) \\ \Delta b_+(y,z) &= [\delta(y+1)-\delta(y)][\delta(z)-\delta(z-1)] \qquad (3.13) \\ \Delta b_-(y,z) &= -\left(\delta(y)+2\sum_{j=1}^{\infty}(-1)^j\delta(y+j)\right)\left(\delta(z)+2\sum_{k=1}^{\infty}(-1)^k\delta(z-k)\right). \end{aligned}$$

Equation (2.16) then gives

$$\begin{aligned} \Delta b_+(u) &= -\delta(u)+2\delta(u-1)-\delta(u-2) \\ \Delta b_-(u) &= -\left(\delta(u)+4\sum_{k=1}^{\infty}(-1)^k k\delta(u-k)\right). \end{aligned} \qquad (3.14)$$

Combining (3.7) and (3.14) then yields

$$\begin{aligned} \Delta c_+(x,t) &= [\gamma(x+1,t)-\gamma(x,t)]\int_{(x-1,x]} \gamma(w,t)\,\mathrm{d}w \\ &\quad -[\gamma(x,t)-\gamma(x-1,t)]\int_{(x,x+1]} \gamma(w,t)\,\mathrm{d}w. \end{aligned} \qquad (3.15)$$

The corresponding expression for $c_-(x,t)$ is omitted due to length.

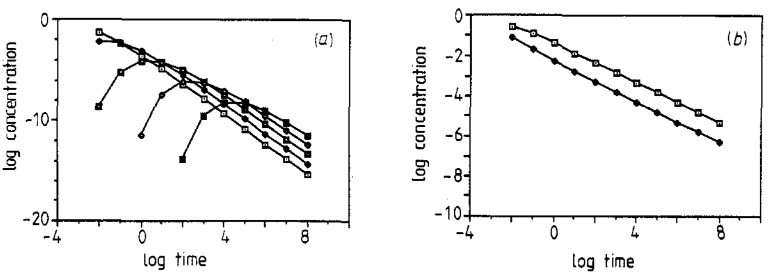

**Figure 2.** In these log-log plots, all logarithms are to the base 2. ($a$) $c_k(t)$ against $t$ for the delta distribution on $R$. $k=1$, 2, 4, 8, 16 on the left from top to bottom. ($b$) $c_+(t)$ (top) and $c_-(t)$ (bottom) against $t$ for the delta distribution on $Z$.

On $Z$, (3.15), (2.6), (2.16) and (3.4) give

$$\begin{aligned}
&\Delta c_+(x,t) = -\exp(-4t)[I_x^2(2t) - I_{x-1}(2t)I_{x+1}(2t)] \sum_{k=-\infty}^{\infty} \delta(x-k) \\
&\Delta c_-(x,t) = (-1)^{x+1}\exp(-6t)I_x(2t) \sum_{k=-\infty}^{\infty} \delta(x-k) \\
&\Delta c_+(Z,t) = -\exp(-4t)[I_0(4t) - I_2(4t)] \\
&\Delta c_-(Z,t) = -\exp(-8t).
\end{aligned} \tag{3.16}$$

On $R$,

$$\Delta c_+(R,t) = -2\,\mathrm{erf}[1/(8t)^{1/2}] + \mathrm{erf}[2/(8t)^{1/2}]. \tag{3.17}$$

Define the combinatorial coefficient $\binom{i}{-1} \triangleq 1$, $i=-1$, and $0$, $i>-1$. For the half-delta distribution on $R$ or $Z$, and $k \geqslant 0$

$$\begin{aligned}
&\beta_k^0(y,z) = \sum_{j=-\infty}^{\infty} \sum_{i=k}^{\infty} 2^{-(i+1)} \binom{i-1}{k-1} \delta(y-j)\delta(z-j-i) \\
&b_-^0(y,z) = \tfrac{1}{2} \sum_{j=-\infty}^{\infty} \delta(y-j)[\delta(z-j) - \delta(z-j-1)].
\end{aligned} \tag{3.18}$$

$b_-$ for the half-delta distribution equals $\frac{1}{2}b_+$ for the delta distribution. The half-delta perturbation $\Delta b_-$ deletes all terms involving $y=0$ or $z=0$ from its $b_-$. Since the delta perturbation $\Delta b_+$ does exactly this to its $b_+$ as well, (3.11) and (3.16) for the delta distribution's $c_+(x,t)$ and $\Delta c_+(x,t)$, when halved, give $c_-(x,t)$ and $\Delta c_-(x,t)$, respectively, for the half-delta distribution. Similar relationships hold between the concentrations $c(t)$.

## 4. The asymptotics of $c(t)$

These asymptotics depend on those of $a(t;u)$. On $Z$, (2.6) and (2.11) give

$$\begin{aligned}
a(t;u) &= 1 - 2\sum_{k=0}^{u-1} \exp(-4t)I_k(4t) - \exp(-4t)I_u(4t) \\
&\sim 1 - (8\pi t)^{-1/2}\left[\left(2\sum_{k=0}^{u-1} 1 + 1\right) - (32t)^{-1}\left(2\sum_{k=0}^{u-1}(4k^2-1) + (4u^2-1)\right)\right] \\
&\sim 1 - \pi^{-1/2}(8t)^{-1/2}(2u+1) + \pi^{-1/2}(8t)^{-3/2}(1/12)(8u^3-2u-3)
\end{aligned} \tag{4.1}$$

(Abramowitz and Stegun 1972, p 377). The asymptotics have been written in a form for later use: descending powers of $t$, followed by factors involving $u$.

On $R$, (2.7) and (2.11) give

$$\begin{aligned}
a(t;u) &= \mathrm{erfc}[u(8t)^{-1/2}] \\
&\sim 1 + 2\pi^{-1/2} \sum_{k=1}^{\infty} (-1)^k \frac{(8t)^{-(2k-1)/2} u^{2k-1}}{(2k-1)(k-1)!} \\
&\sim 1 - \pi^{-1/2}(8t)^{-1/2} 2u + \pi^{-1/2}(8t)^{-3/2} \tfrac{2}{3} u^3
\end{aligned} \tag{4.2}$$

(Abramowitz and Stegun 1972, p 297).

Let $\boldsymbol{b}(v)$ be the Fourier transform (Lighthill 1978, p 15) of a given distribution $b(u)$. Then the $k$th moment of the distribution $b$ is

$$\mu_k(b) \triangleq \int u^k b(u)\,\mathrm{d}u = \left(\frac{1}{2\pi\mathrm{i}}\frac{\partial}{\partial v}\right)^k_{v=0} \boldsymbol{b}(v) \tag{4.3}$$

where the subscript $v=0$ indicates evaluation at 0. The preceding, and equations (2.14) and (2.16), relate the asymptotics of $c(t)$ and $\Delta c(M, t)$ to the moments of distributions determined by the placement of the initial monomers.

If the distances between consecutive monomers $\ldots, P_{-1}, P_0, P_1, \ldots$ are independently and identically distributed, the monomers are said to be in a renewal distribution (Bailey 1964, p 223). The above results simplify for a renewal distribution. Let $f_k(u)$ between the density function for the distance between any pair $P_l$ and $P_{k+l}$ in such a renewal. For consistency, define $f_0(u) \triangleq \delta(u)$. By the definition of $\beta_k$ following (2.1)

$$\beta_k(y, y+u) = c_1(y, t_0) f_k(u). \tag{4.4}$$

Define $m_k \triangleq \mu_k(f_1)$ to be the $k$th moment of the distance between the monomers. Equations (2.16) and (4.4) give

$$\beta_k(u) = c_0 f_k(u) = m_1^{-1} f_k(u) \tag{4.5}$$

since the concentration of monomers is the reciprocal of the average distance between them.

Because $f_k$ is the $k$th convolution of $f_1$ for a renewal distribution, the Fourier transform of $f_k$ has a convenient property (Bailey 1964, p 225):

$$\boldsymbol{\beta}_k(v) = m_1^{-1}\boldsymbol{f}_k(v) = m_1^{-1}\boldsymbol{f}_1^k(v). \tag{4.6}$$

$\boldsymbol{f}_1^k(v)$ is the $k$th power of $\boldsymbol{f}_1(v)$.

Equations (2.3)-(2.5) and (4.6) then give

$$\begin{aligned} \boldsymbol{b}_k(v) &= m_1^{-1}\boldsymbol{f}_1^{k-1}(v)[1-\boldsymbol{f}_1(v)]^2 \\ \boldsymbol{b}_+(v) &= m_1^{-1}[1-\boldsymbol{f}_1(v)] \\ \boldsymbol{b}_-(v) &= m_1^{-1}\frac{1-\boldsymbol{f}_1(v)}{1+\boldsymbol{f}_1(v)}. \end{aligned} \tag{4.7}$$

Hence, for renewal distributions, on either $Z$ (4.1) or $R$ (4.2), equations (2.14), (4.3) and (4.7) give the following:

$$\begin{aligned} c_k(t) &\sim (4/\sqrt{\pi})(8t)^{-3/2}[(k-1)m_1^2 + m_2] \\ c_+(t) &\sim (2/\sqrt{\pi})(8t)^{-1/2} \\ c_-(t) &\sim (1/\sqrt{\pi})(8t)^{-1/2} \end{aligned} \tag{4.8}$$

since $\mu_0(b_k) = \mu_1(b_k) = 0$ and $\mu_0(b_+) = \mu_0(b_-) = 0$. For lattice distributions (Feller 1971, p 138), e.g. distributions on $Z$, $|\boldsymbol{f}_1(v)| = 1$ for some $v$, so the summation of the infinite geometric series implicit in (4.7) for $b_-$ must, and probably can, be justified by continuity arguments for generalised functions (Lighthill 1978, p 28). Equations (4.8) correct errors in the final two equations of I. Figure 2 demonstrates the asymptotic relationships implied by (4.8).

## 5. Periodic, absorbing or reflecting boundary conditions

The boundary conditions present only a few conceptual difficulties and can be handled by the principle of reflection. Naively, one might expect that the boundary condition solutions might superpose appropriate reflections of either the polymer concentrations or the initial monomer positions. In fact, as (2.1) shows, the concentrations in Ppoly depend on events involving monomer pairs; as a consequence, the appropriate reflections take place in two dimensions, where they can account for paired interactions.

We consider first the periodic media, $Z(\bmod L)$ (periodic lattices of $L$ points) and $R\ (\bmod L)$ (circles of length $L$). The reader may wish to reread § 2 up to the paragraph preceding (2.9).

As before, the relevant aspects of the initial monomer distribution are specified by $\beta_k(y, z)$. For a physically realistic monomer distribution on a periodic medium, only a finite number, say $N$, of monomers occur in a particular realisation of the initial distribution. This realisation contributes 0 to $\beta_k(y, z)$ for $k \geq N$. On $Z\ (\bmod L)$ and $R\ (\bmod L)$, each point is given an infinite number of coordinates, separated from one another by multiples of $L$. In order to get a unique representation of the initial monomer distribution, we define $\beta_k(y, z) \triangleq 0$, unless $0 \leq y < L$ and $0 \leq z - y < L$.

Equation (2.1) required a definition of a leftmost monomer in a polymer. The definition given there for infinite media can fail on a periodic medium, especially when all the monomers are in a single polymer. Even on a periodic medium, however, every polymer contains exactly one monomer which never met a polymer coming from the left. This yields a definition of leftmost monomers consistent with the definition for infinite media, and holding for periodic media as well.

This definition allows $c_k(x, t)$ to retain its interpretation as a probability (preceding (2.1)). The events $A$ of (2.1) must be slightly modified, e.g. $A_0$ must include another condition: (c) if the medium is periodic, $P_0$ is the leftmost monomer in the polymer (i.e. $P_0$ met $P_{k-1}$ as $P_{k-1}$ came from the right). As will be shown next, on $Z\ (\bmod L)$ or $R\ (\bmod L)$, the annihilation function is given by

$$a_L(x, t; y, z) = \sum_{p=0}^{\infty} [a_\infty(x, t; y - pL, z + pL) - a_\infty(x, t; z - pL - L, y + pL + L)] \tag{5.1}$$

where $a_\infty(x, t; y, z)$ is the annihilation function for the corresponding infinite medium, $Z$ or $R$, given implicitly by (2.6)-(2.8).

Equation (5.1) can be demonstrated as follows (see figure 3($a$)): let the initial position of the relevant monomers $P_0$ and $P$ be $y$ and $z$, where $0 \leq y < L$ and $0 \leq z - y < L$. In the definition of the events $A$ preceding (2.1), *$P$ must now meet $P_0$ as $P$ comes from the right, not from the left.*

The demonstration follows the proof of (2.8), but here the diffusing point starts at $(y, z)$ in the parallelopiped bounded by the lines $Y = 0$, $Y = L$, $Z - Y = 0$ and $Z - Y = L$, and finishes at time $t$ on one of two paired half-lines starting from $(x, x)$. The italicised restriction above is equivalent to the following: *if the point ever passed through the line $Z - Y = L$, it passed through the line $Z - Y = 0$ first.*

Reflections give an interpretation to the individual terms in (5.1): they correspond to sources of diffusive points of alternating sign +, −, +, ... at $(y, z)$, $(z - L, y + L)$,

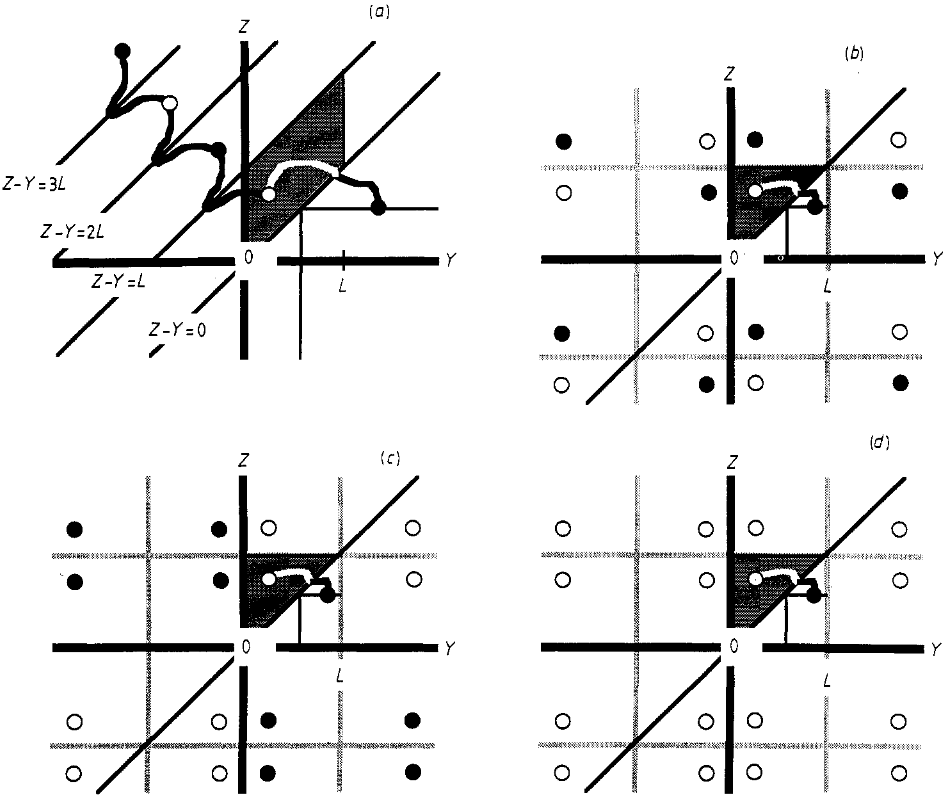

**Figure 3.** These reflections provide solutions for various boundary conditions on $(0, L)$. Positive sources are in white; negative, in black. The two-dimensional diffusions can start anywhere in the shaded areas and can end anywhere on the black half-lines. A sample diffusive path is shown in each case. ($a$) Periodic. Because cancellation of diffusive points occurs at the lines $Z-Y=0$, $Z-Y=L$, $Z-Y=2L, \ldots$, the sample diffusive path represents those paths which cross $Z-Y=0$ before they cross $Z-Y=L$. ($b$) Absorbing boundaries at position 0 and position $L$: diffusive points are cancelled on the square with vertices $(0, 0)$, $(0, L)$, $(L, 0)$ and $(L, L)$. ($c$) Absorbing boundary at position 0 and reflecting boundary at position $L$: diffusive points are cancelled on the line segments joining $(0, 0)$ to $(0, L)$ or $(L, 0)$. There is no diffusive flux across the line segments joining $(L, L)$ to $(0, L)$ or $(L, 0)$. ($d$) Reflecting boundaries at position 0 and position $L$: there is no diffusive flux across the square with vertices $(0, 0)$, $(0, L)$, $(L, 0)$ and $(L, L)$.

$(y-L, z+L), \ldots$. There is one source between each pair of lines $Z-Y=qL$ and $Z-Y=qL+L$, $q=0, 1, 2, \ldots$. Diffusive points arriving at the paired half-lines from the source between the lines $Z-Y=qL$ and $Z-Y=qL+L$ either (a) passed through $Z-Y=qL$ before passing through $Z-Y=qL+L$ or (b) passed through $Z-Y=qL+L$ before passing through $Z-Y=qL$. The cancellation of diffusive points occurring at $Z-Y=qL$, $q=1, 2, 3, \ldots$, ensures that the sum in (5.1) equals $a_L(x, t; y, z)$.

Because the points of $Z \pmod L$ and $R \pmod L$ have an infinite number of coordinates, separated from one another by multiples of $L$, the concentrations $c(x, t)$ at a point must be summed over all of its coordinates $\ldots, x-L, x, x+L, \ldots$, to give the total concentration at that point. For finite $L$, (2.14) continues to hold, if $1/L$ replaces $1/2P$ in (2.10). $\beta_k(u)=0$ outside $[0, L)$, because $\beta_k(y, z) \triangleq 0$, unless $0 \leq y < L$ and $0 \leq z-y < L$, so only values of $a(t; u)$ within $[0, L)$ are relevant.

Substituting both sides of (5.1) into (2.10) gives a relation between $a_L(t;\, u)$ and $a_\infty(t;\, u)$, the spatially averaged annihilation functions for a periodic medium ($Z$ (mod $L$) or $R$ (mod $L$)) and its corresponding infinite medium ($Z$ or $R$):

$$a_L(t;\, u) = \sum_{p=0}^{\infty} [a_\infty(t;\, u+2pL) - a_\infty(t;\, 2L-u+2pL)]. \tag{5.2}$$

Equation (5.2) has also been proved directly by reflection (Balding 1988). Equation (5.2) can be used in conjunction with (2.14) to derive known results (Torney and McConnell 1983, Balding 1988) for periodic media.

Absorbing or reflecting boundary conditions are easy by comparison (figures 3($b$)-($d$)). Without loss of generality, let the interval defined by the boundary conditions be $(0, L)$, where $L$ may be infinite. Unlike the case of periodic media, there is no complication in the definition of leftmost monomers, but the ranges of integration in the two integrals defining the annihilation Green function of (2.8) become $\{0, x]$ and $(x, L\}$, where the brackets '{' and '}' represent either closed or open endpoints, depending on the boundary conditions. With this modification, let (2.8) continue to give the annihilation functions $a(x, t;\, y, z)$ even when $z \leq y$. This continuation ensures the correct conditions of zero concentration or zero flux of diffusing monomers at $Y=0$, $Z=0$, $Y=L$ and $Z=L$.

Paper I gives a discussion of the many other problems which can be solved with the method of (2.1).

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