One-dimensional Brownian motion with an accumulating boundary: Asymptotic results

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We consider one-dimensional Brownian motion with an accumulating boundary, i.e., an absorbing boundary that grows through the mechanical accumulation of absorbed particles. We show that the diffusion-equation (DE) description of the boundary-growth process is internally inconsistent at short times. Accordingly, we consider this problem in the context of a model that caricatures the Fokker-Planck description in position-velocity space. Asymptotic results for both short and long times are obtained for the model and the former are shown to be internally consistent. The DE predicts that the boundary grows as $t^{1/2}$ for all time, whereas the model reproduces this result only for long times while predicting an initial growth proportional to t. We also obtain a lower bound and an upper bound on the boundary growth predicted by the model description that are valid for all times. An approximation in which the solution for a fixed absorbing boundary is used with the boundary-growth equation is also discussed in Appendixes B and C.

I. INTRODUCTION

There has been considerable interest in recent years in diffusive-growth processes.[1] A common element of the theory that has developed is the diffusion equation (DE) or, in lattice systems, a related random walk description. Since growth processes are inherently a boundary phenomenon, the use of the DE in describing these is subject to the same concerns as generally apply in such situations.[2–4] For the relatively simple case of Brownian motion with a fixed absorbing boundary it has been shown[2–4] that the DE is inadequate in both the space and time boundary layers. We would anticipate that a similar situation exists in the more complicated case of an accumulating boundary at which diffusive growth occurs.

The purpose of this paper is to examine the simplest-appearing possible case of diffusive growth, one-dimensional Brownian motion with an accumulating boundary, and to compare the DE results with those obtained for a simple model[4] that correctly treats the boundary condition at the growing interface. We have only been able to obtain asymptotic results in the case of the model; however, these enable us to describe the initial layer and confirm the expected long-time transition to diffusive behavior. We find that the initial growth is proportional to t in contradistinction to the DE result which predicts an interface growth proportional to $t^{1/2}$ for all time. We also show that the model is internally consistent at short times, whereas the DE fails in this regard also. By the use of a fairly simple physically motivated argument we are able to obtain bounds on the boundary growth that indicate a complicated dependence on time outside the asymptotic regions. (Additional bounds are discussed in Appendix C for an approximate solution based on using the fixed-boundary solution for the particle density and current to determine the interface growth.) This approximation is also used in Appendix B to obtain a solution for the related Stéfan problem in which the growing interface separates two distinct phases with the interface density specified. Interestingly, the Stéfan problem turns out to be much simpler to solve, in principle, than the accumulating boundary problem.

The results we have obtained indicate that diffusion-controlled growth processes can only be fully understood in the context of a theoretical framework that correctly describes the boundary condition at the growing interface.

II. DIFFUSION-EQUATION THEORY

Consider a one-dimensional system of Brownian particles which at $t=0$ is uniformly distributed in the half-space $x>0$. The interface boundary, initially at $x=0$, accumulates all incident particles thereby extending the interface into the region $x>0$ with increasing time. For convenience we denote the Brownian particles position x at the particles' "leading edge" and the particles will be assumed to have size r_0. This moving-boundary problem is readily described; however, we have been unable to find any discussion of this problem in any of the excellent general treatments of Brownian motion[5,6] that extend the DE description. For specific applications related results have been obtained within this context, however.[7,8]

The DE and interface equation of motion are

$$\frac{\partial n}{\partial t}=D\frac{\partial^2 n}{\partial x^2},\quad n(x,0)=n_0,\quad n(x_B(t),t)=0\ , \tag{1}$$

$$x_B(t)=r_0\int_0^t dt'D\frac{\partial n}{\partial x}\bigg|_{x_B(t')}\ , \tag{2}$$

where $(-D\partial n/\partial x)_x$ is the particle flux at x; the negative sign does not occur in (2) since the integral represents the accumulated number of particles incident at the interface in the interval $(0,t)$. A particular solution to (1) that satisfies the initial condition is

$$n=n_0-A\,\mathrm{erf}[x(4Dt)^{-1/2}]\ . \tag{3}$$

This implies that

$$n_0 = A\ \mathrm{erf}[x_B(t)/(4Dt)^{1/2}] \tag{4}$$

or that $x_B(t) = C(4Dt)^{1/2}$. Equating the latter result to that obtained from (2) we find, with (3),

$$A = e^{C^2}\frac{C}{r_0} = \frac{n_0}{\mathrm{erf}C}\ , \tag{5}$$

which uniquely determines the constants A and C. A plot of $Ce^{C^2}\mathrm{erf}C$ versus C is given in Ref. 8. The growth law predicted by the DE is $x_B(t) \propto t^{1/2}$, i.e., both $x/(4Dt)^{1/2}$ and $x_B(t)/(4Dt)^{1/2}$ are similarity variables. The growth law is universal in the sense that it holds for all values of time. In what follows we will find that this universality is not valid for the case of a model which more accurately prescribes the interface-boundary condition.

III. MODEL FOKKER-PLANCK EQUATION

The proper boundary condition at the interface is that only the emergent particle density vanishes. This implies that the theoretical framework must permit a distinction between incident and emergent particles or, more generally, that this framework include both the Brownian-particle position and velocity. Considerable attention has been given to such a theory for the case of an absorbing boundary.[2-4] Here we will use a model that appears to caricature the Fokker-Planck equation[9] (FPE) and which we have used earlier[4,5] to describe absorbing boundary problems.[10] This model permits velocities $\pm\alpha$ so that the distribution functions $u_2(x,\alpha,t)$ and $u_1(x,-\alpha,t)$ replace $n(x,t)$ in providing the basic description. The u_i satisfy equations

$$\frac{\partial u_i}{\partial t} + (-1)^i \frac{\partial u_i}{\partial x} = \beta(u_1 - u_2)(-1)^i, \quad i = 1,2 \tag{6}$$

where β plays the role of the friction coefficient in the FPE.[10] This model corrects the two distinct shortcomings inherent in the DE description. In addition to allowing the boundary condition to match the actual physical process, the model also leads to the telegraphers equation for the density, $u_1 + u_2$, which has a finite signal speed. Since the breakdown of the DE at short times results from its characteristic infinite signal speed, the model represents a major qualitative improvement in this regard. In the concluding part of Sec. IV we show that at long times the model and DE results are identical, and so we expect that the model provides a more realistic description than the DE over the entire space-time domain.

In Appendix A we show that this model can be viewed in another light which has an interpretation in terms of an approximation to the solution of the FPE containing the full range of particle velocities. This point provides added motivation for the use of the model, and a basis for its generalization, but this is a separate issue that will not be pursued here.

The general solution to (6) satisfying the initial conditions $u_i(x,0) = u_0$, $i = 1,2$ is most conveniently expressed in terms of $w = u_1 + u_2$ and $v = u_2 - u_1$; denoting Laplace transform by an overbar we have[4]

$$\overline{w}(x,s) = \frac{2u_0}{s} + \overline{A}(s)e^{-qx}\ , \tag{7a}$$

$$\overline{v}(x,s) = \frac{s^{1/2}}{(s+2\beta)^{1/2}}\overline{A}(s)e^{-qx}\ , \tag{7b}$$

where $q \equiv [s(s+2\beta)]^{1/2}\alpha^{-1}$. These transforms can be inverted[4] but in order to use the time-domain representation to find an analytic result for $x_B(t)$ valid for all times requires solving a complicated integral equation for $A(t)$ which we have been unable to do. The above results do allow us to obtain asymptotic results for both small and large values of the time and in addition to their own intrinsic interest the former result will also provide us with a basis for examining the self-consistency of the model.

The above equations must be complemented by the boundary condition that specifies the interface motion. This is found by considering a mass (or particle) balance for the system. We find

$$\dot{x}_B(t) = -\frac{v(x_B(t),t)\alpha r_0}{1 - r_0 w(x_B(t),t)} = \frac{w(x_B(t),t)\alpha r_0}{1 - r_0 w(x_B(t),t)}\ , \tag{8}$$

where we have made use of the physically correct relationship characterizing the interface, $w = -v$. Note that in the DE description the negative term in the denominator on the right-hand side (rhs) is not present because of the interface-boundary condition of vanishing interface density. The DE cannot self-consistently provide information regarding the interface density. Here this information, in principle, can be determined leading to the more complicated equation above. In looking for asymptotic results we anticipate having only to consider the leading (small) terms contributing to w, and therefore we can approximate the above result by replacing the denominator by 1. The exact expression for $\dot{x}_B(t)$ is considerably more complicated than the corresponding expression that occurs in the one-dimensional Stéfan problem[8] in which the growing interface separates two phases and the interface density is specified; this problem is briefly discussed in Appendix B.

IV. ASYMPTOTIC RESULTS

We first consider the small-time case and assume

$$A(t) = a_0 + \sum_{i=1}^{\infty} a_i t^{k_i}\ , \tag{9}$$

where $0 < k_1 < k_2 < \cdots$. Expanding (7), with (9), in descending powers of the transform variable and inverting we find

$$x_B(t) = \alpha u_0 r_0 t + O(t^{k_1+1}) \tag{10}$$

subject to the obvious constraint $u_0 r_0 < 1$ which is always realized in a physical system. This result predicts a much faster initial growth than that predicted by the DE and is our primary finding.

Since the model equation description reduces to the DE description at long time[4] we may anticipate a similar result in the present specific case. At long times $q \cong s^{1/2}(2\beta)^{1/2}/\alpha$ and

$$\overline{w} \cong 2u_0/s + \overline{A}(s)e^{-s^{1/2}(2\beta)^{1/2}x/\alpha} , \tag{11a}$$

$$\overline{v} \cong \frac{\overline{A}(s)}{(2\beta)^{1/2}} s^{1/2} e^{-s^{1/2}(2\beta)^{1/2}x/\alpha} , \tag{11b}$$

and if we note that $D = \alpha^2/2\beta$ for the model and that the particle flux is $j = \alpha v$, then the relationship $j = -D\partial w/\partial x$ (Fick's Law) is seen to hold at long times. Since we can expand $A(s)$ in a descending series as

$$\overline{A}(s) = \sum_{n=0}^{\infty} (a_n s^{n-1} + s^{e-1} b_n s^n) , \tag{12}$$

with $0 < e < 1$ it follows that at x_B, where $w + v = 0$, inverting (11) and retaining the dominant large-t term gives $w_B(x_B(t),t) = 0$; note, the inverse must be taken first and then x set equal to $x_B(t)$. Equation (11a), the Fick's-law relationship for the flux, and the above interface-boundary condition are identical to the corresponding relationships in the DE theory and thus $x_B(t)$ is identical to the DE result at long times.

V. CONCLUDING REMARKS AND OBSERVATIONS

The major result we have found is that the initial interface growth occurs much faster than predicted by the DE. The DE result leads to the conclusion that for all time the ratio

$$N_B(t)/N_0(t) = C\pi^{1/2}/n_0 r_0 ,$$

where $N_0(t)$ is the number of particles absorbed at a fixed boundary at $x = 0$ and $N_B(t)$ is the number accumulated in the region $0 < x < x_B(t)$ in the interval $(0,t)$. This ratio is constant for all time, and since $r_0 n_0 \leq 0.56\pi^{1/2}$, C can take on values[8] such that ratio is greater than 1 as $t \to 0$. For the model we can show[11]

$$N_0(t) = u_0 \frac{\alpha}{\beta} [\Phi(-\tfrac{1}{2}, 1; -2\beta t) - 1] \tag{13a}$$

$$\cong u_0 \alpha t \quad \text{as } t \to 0 \tag{13b}$$

(Φ is a confluent hypergeometric function) which gives the correct limiting form $N_B(t)/N_0(t) = 1$ as $t \to 0$. Thus the DE description is not only incorrect at small times, as is well known, but it is internally inconsistent as well, whereas the model provides a more accurate description which is also self-consistent.

We next briefly consider bounds on $x_B(t)$; further consideration of this subject follows in Appendix C. The lower bound

$$N_0(t) r_0 \leq x_B(t) \tag{14}$$

is obvious. The point $x^* = r_0 N_0(t)$ initially has $2u_0 r_0 N_0(t)$ particles located to its left. In the interval $(0,t)$ the particles that are accumulated come from either this group, the group initially in the segment $x^*(t) \leq x \leq x^{**}(t)$, where $x^{**}(t) \equiv x^*(t) + r_0[2u_0 r_0 N_0(t)]$ or from particles initially to the right of $x^{**}(t)$. In the latter case the particles that are accumulated in $(0,t)$ must pass $x^{**}(t)$ moving to the left. Not all of these latter particles, or the particles initially to the left of $x^{**}(t)$, are accumulated in $(0,t)$, thus

$$x_B(t) \leq 2u_0 r_0 x^{**}(t) + r_0 N_0(t)$$
$$2u_0 r_0 x^{**}(t) + r_0 N_0(t) = N_0(t) r_0 (1 + 2u_0 r_0 + 4u_0^2 r_0^2) . \tag{15}$$

We conclude with two observations. The first of these relates to the approximation in which x_B is determined from (8) by using the solution for a fixed absorbing boundary at $x = 0$ in place of that for an accumulating boundary.[7] For this approximation to be of value it would have to be embedded in a formal scheme, e.g., as the lowest-order solution in a multiple-scale expansion. Obtaining an analytical solution, even in lowest order, appears to be a formidable task; however, numerical results could be found directly using the results of Ref. 4. In Appendix B we utilize this approximation to find a solution for the Stéan problem;[8] our initial assumption that the accumulating-boundary-layer problem was the simplest example of diffusive growth that could be considered turns out to be false and we will see that the Stéfan problem is, in principle, simpler and, in the context of the approximation described above, exactly solvable. Our second, and concluding observation pertains to the use of this approximation with Eq. (8) to find improved bounds for x_B. The properties of the confluent hypergeometric functions[12] are particularly well suited to this task and such results would serve an important role as part of a theory which puts the approximation on a more rigorous basis. In Appendix C we briefly outline how such bounds might be developed.

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APPENDIX A: "DERIVATION" OF EQ. (6) FROM THE FPE

The model FPE, Eq. (6), expressed in terms of the variables $w = u_2 + u_1$ and $v = u_2 - u_1$, is

$$\frac{\partial w}{\partial t} + \alpha \frac{\partial v}{\partial x} = 0 , \tag{A1a}$$

$$\frac{\partial v}{\partial t} + \alpha \frac{\partial w}{\partial x} = -2\beta v . \tag{A1b}$$

Note that for the model w and αv are, respectively, the particle density and current.

If we consider solutions of the full FPE of the form $f(x,v,t) = f_i(x,v,t)$ with $i = 1,2$ according to whether $v < 0$ or $v > 0$ and take

$$f_i(x,v,t) = \frac{e^{-v^2/2kT}}{(2\pi kT)^{1/2}} \sum_{i=0}^{\infty} a_{in}(x,t) H_{in}(v) , \tag{A2}$$

where $H_{in}(v)$ are a suitable chosen set of orthogonal half-range polynomials in $\pm v$, then the lowest-order approximation is

$$f_i(x,v,t)=n_i(x,t)\frac{e^{-v^2/2kT}}{(2\pi kT)^{1/2}} , \tag{A3}$$

where we have called $a_{i0}=n_i$, i.e., separate local Maxwellians for $v \lessgtr 0$. If the n_i are determined by the moment equations obtained by multiplying the FPE by 1 and v followed by integration over v we obtain[13]

$$\frac{\partial M_0}{\partial t}+\frac{\partial M_1}{\partial x}=0 , \tag{A4a}$$

$$\frac{\partial M_1}{\partial t}+kT\frac{\partial M_0}{\partial x}=-\zeta M_1 , \tag{A4b}$$

where $M_0=\frac{1}{2}(n_1+n_2)$, $M_1=(n_2-n_1)(kT/2\pi)^{1/2}$, and ζ is the friction coefficient. Equations (A1) and (A4) are equivalent, allowing the solutions of the former to be interpreted in terms of an approximate solution to the FPE. This correspondence is similar to that between solutions of the simple Bhatnager-Gross-Krook (BGK) model Boltzmann equation and approximate solutions of the linearized Boltzmann equation[14] although in the present case the correspondence is at a decidedly reduced level of detail.

APPENDIX B: APPROXIMATE SOLUTION OF THE STÉFAN PROBLEM

The approximation in which solutions for w and v for a fixed interface are used in the interface equation of motion leads to an immediate solution of the Stéfan problem.[8] Here we consider the interface to be separating two phases with diffusion occurring in only one of these. The density of the fixed phase will be denoted by w^I; initially this phase occupies the region $-\infty < x < 0$. The interface density w^0 is determined by the conditions of local equilibrium at the interface. The density of the diffusing phase, initially occupying the region $0<x<\infty$, is the quantity we have to find, $w(x,t)$, for $t>0$ after the two phases have come into contact and the interface growth has begun.

The DE solution of this problem follows along the same lines as the treatment of Sec. II; in particular, $x_B(t)\propto t^{1/2}$ for all time. In the context of the model FPE the interface equation of motion is greatly simplified relative to Eq. (8),

$$x_B(t)=-\alpha v(x_B,t)/(w^I-w^0) . \tag{B1}$$

We obtain an approximate solution by replacing $v(x_B,t)$ with $v(0,t)$ with the latter determined for a fixed interface. This latter quantity follows directly from our previous results[4] for an absorbing boundary with appropriate changes to incorporate the changed boundary condition $w(0,t)=w^0$,

$$v(0,t)=[w^0-w(x,0)]e^{-\beta t}I_0(\beta t) , \tag{B2}$$

where I_n is a modified Bessel function. We then have, subject to our earlier caveats concerning this approximation,

$$x_B(t)=\frac{[w(x,0)-w^0]}{w^I-w^0}\alpha t e^{-\beta t}[I_0(\beta t)+I_1(\beta t)] . \tag{B3}$$

At long times we again recover the DE result, at short times we again have a linear dependence on time, and the transition involving the sum of two Bessel functions is relatively complicated.

APPENDIX C: BOUNDS FOR $x_B(t)$

We want to briefly outline here a procedure for obtaining bounds on x_B as determined from Eq. (8) with $w(x_B(t),t)$ replaced by $w(x_B(0),t)$, the model equation solution for a fixed absorbing boundary. For this approximation $w(x_B(0),t)=w(0,t)$ as determined previously[4]

$$w(0,t)=(2/\pi)u_0\Phi(\tfrac{1}{2};2;-2\beta t) . \tag{C1}$$

Since $\Phi(\frac{1}{2};2;-x)\le\Phi(-\frac{1}{2};1;-x)$ follows directly from the Kummer transformation

$$\Phi(a;b;-x)=e^{-x}\Phi(b-a;b;x)$$

and the definition of the Φ's, and since[12]

$$\Phi'(a;b;x)=(a/b)\Phi(a+1;b+1;x)$$

we find in this approximation

$$x_B(t)=\int_0^t dt'(2\alpha/\pi)r_0u_0\frac{\Phi(\frac{1}{2};2;-2\beta t')}{1-(2/\pi)u_0r_0\Phi(\frac{1}{2};2;-2\beta t')} \tag{C2a}$$

$$\le\int_0^t dt'(2\alpha/\pi)r_0u_0\frac{\Phi(\frac{1}{2};2;-2\beta t')}{1-(2/\pi)u_0r_0\Phi(-\frac{1}{2};1;-2\beta t')} \tag{C2b}$$

$$\le 2(\alpha/\beta)\ln\{[1-(2/\pi)u_0r_0]/[1-(2/\pi)u_0r_0\Phi(-\tfrac{1}{2};1;-2\beta t)]\} . \tag{C2c}$$

This bound can be improved by using the recursion relation[12] $\Phi(\frac{3}{2};3;-2\beta t)+\Phi(\frac{1}{2};3;-2\beta t)=\Phi(\frac{1}{2};2;-2\beta t)$ in the numerator of (C2a), directly integrating the term containing $\Phi(\frac{3}{2};3;-2\beta t)$, and repeating the foregoing procedure with the remaining term to arrive at a new inequality. Similarly, lower bounds can be obtained by using the inequality $\Phi(\frac{3}{2};3;-x)\le\Phi(\frac{1}{2};2;-x)$ in the numerator of (C2a), again obtaining an exact differential. In the case of the lower bound it is likely that the expression obtained by simply neglecting the second term in the denominator of (C2a) will provide the strongest result. As discussed earlier, a more detailed study of these bounds using the approximation (B3) in (8) is only warranted in the context of a more precise theory incorporating that approximation.

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