Steady, two-dimensional Brownian motion with an absorbing boundary

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We consider steady Brownian motion in the infinite strip with boundaries at $x=0, x=L$, with the latter absorbing. Our specific interest is to obtain insight into how a prescribed "far away" density at $x=0$ is mapped onto the absorbing boundary. The diffusion equation description cannot address this problem; instead we utilize an approximate solution of the Fokker-Planck equation. The major result we obtain is qualitative—that there may exist points or regions along the boundary where absorption takes place to a greater (or lesser) extent than might be inferred from the given far away data. A specific example illustrating this point is included.

I. INTRODUCTION

One-dimensional (1D) Brownian motion with an absorbing boundary has been the subject of a number of recent studies.[1–5] The focus of attention in these has been to improve the treatment at the boundary provided by the macroscopic description in which the density is considered to vanish. In order to properly treat this problem it is necessary to include both the Brownian particle velocity and position as independent variables, allowing the incident and emergent particle densities to be separately specified at the boundary where only the latter vanishes. Then the macroscopic density $n(x)$ satisfying the diffusion equation (DE) is replaced by the phase-space density $f(x,v)$ which satisfies the Fokker-Planck equation (FPE). The solution of the FPE with the boundary condition $f(L,v)=0$, $v<0$ corresponding to steady one-dimensional Brownian motion on the line $0\le x\le L$ with absorption at $x=L$ has been obtained by a number of approximate techniques[3–5] and subsequently an exact, formal solution in terms of an eigenfunction expansion has also been found.[1,2] The basic questions regarding the behavior of the solution at the boundary have been largely resolved as a result of these studies.

In the present paper we consider the absorbing boundary problem for the case where there are two independent space variables.[6] Here a further shortcoming of the DE description becomes manifest since this cannot provide any information concerning the variation in density along the absorbing boundary, e.g., if there are points or regions on the boundary where the absorption of particles occurs to a greater (or lesser) extent than might be expected. Since the DE requires that the density vanish along the entire boundary regardless of the prescribed "far away" density we have no basis (other than computer simulation) for generating such expectations. For this reason an approximate treatment of this problem in the context of the FPE would be especially useful in providing some qualitative insights regarding possible expectations.

The specific problem we consider here will be Brownian motion in the infinite strip $-\infty<y<\infty$, $0\le x\le L$, where the system is prescribed along $x=0$ and absorbed along $x=L$. The boundary conditions will include the far away density $n(0,y)=\int d\mathbf{v}\, f(0,y,\mathbf{v})$ and the absorption condition $f(L,y,\mathbf{v})=0$, $v_x<0$, $-\infty<v_y<\infty$. Our primary interest will be to determine how the density $n(0,y)$ is mapped onto the boundary $x=L$ by the FPE. Aside from its intrinsic interest, we believe that this problem has application in a number of areas of current interest including the development of fractal structures in diffusion-limited aggregation,[7] the deposition of metallic vapors on substrate surfaces,[8] and a variety of biophysical situations.[9] Although we have chosen the simplest possible two-dimensional geometry for this preliminary study, the extension to other geometries as well as to systems where the host fluid is in motion should also be possible.

As mentioned above, our primary interest will be in determining the density $n(L,y)$ obtained for steady two-dimensional Brownian motion in an infinite strip with absorption at $x=L$. In Sec. II we formulate this problem utilizing the bimodal Maxwellian moment method of Lees[10] that we used earlier in treating one-dimensional problems.[5,6] In Sec. III we solve the governing moment equations by making use of an expansion in the inverse friction coefficient. This latter approximation is necessitated by the increased difficulty in finding an "exact" solution to the moment equations in two dimensions. A discussion of our results, including some implications regarding the boundary behavior, follows in Sec. IV. In the Appendix we examine the use of the high friction coefficient expansion in the context of a model FPE by comparing the expanded exact solution with the solution of the expanded equations and showing that these are identical.

II. FORMULATION

To begin we summarize the DE result for the specific problem being considered. The DE together with boundary conditions forms the elliptic system

$$\nabla^2 n(x,y)=0\ , \tag{1}$$

$$n(0,y)\equiv n(0),\quad n(L,y)=0\ ,$$

$$0\le x\le L,\quad -\infty\le y\le\infty$$

which has solutions

$$\bar{n}(x,q)=\bar{n}(0)(1-e^{-2ql})^{-1}(e^{qx}-e^{q(2L-x)}) , \tag{2a}$$

$$n(x,y)=\frac{\sin}{2L}(\pi x/L)\times\int dy' n(0,y')\left[\cosh\left[(y-y')\frac{\pi}{L}\right]-\cos\left[\pi\frac{x}{L}\right]\right]^{-1} , \tag{2b}$$

in Fourier (x,q) and physical (x,y) space representations. As stressed above, this result is unsatisfactory along $x=L$ since the absorbing boundary conditions precludes gaining any insights regarding possible preferential absorption regions on the boundary.

The FPE for steady two-dimensional Brownian motion in the geometry being considered is

$$\left[v_x\frac{\partial}{\partial x}+v_y\frac{\partial}{\partial y}\right]f(x,y,v_x,v_y)=\zeta\frac{\partial}{\partial v}\left[\alpha\frac{\partial}{\partial \mathbf{v}}+\mathbf{v}\right]f(x,y,v_xv_y) , \tag{3}$$

where $\alpha\equiv kT/m$, ζ is the friction coefficient, and the steady-state distribution function f is a function of both the Brownian particle position and velocity. This description allows us to accurately prescribe the boundary condition along $x=L$, which is

$$f(L,y,v_x,v_y)=0,\quad v_x<0 . \tag{4}$$

Solving (3) subject to (4) together with related boundary conditions poses a more difficult problem than is encountered in the corresponding one-dimensional case. Our approach will be to make use of the method of Lees[10] that we used earlier with success in studying the one-dimensional case together with some additional assumptions that will allow us to deal with the increased difficulty inherent in solving a system of partial differential equations (2D) instead of ordinary differential equations (1D). We begin by assuming that for $v_x \lessgtr 0$ f can be represented by separate partially linearized local Maxwellian distribution functionals where the unknown parametric functions are to be determined:

$$f_i(x,y,v_x,v_y)=\frac{n_i(x,y)}{2\pi\alpha}\left[1+\frac{v_x u_i(x,y)}{\alpha}+\frac{v_y w(x,y)}{\alpha}\right]e^{-v^2/2\alpha} , \tag{5}$$

with $i=1,2$ according to whether $v_x>0$, $v_x<0$. The unknown functions n_i,u_i,w are determined by using (5) to express the moments of f as functionals of these quantities and then solving the moment equations generated from (3). It is important to note that the significance of f here is through its role in generating moments and we will limit our attention to this aspect of the solution in what follows.

The moments of f are defined as

$$M_0=\int d\mathbf{v}\, f ,\quad M_\alpha=\int d\mathbf{v}\, v_\alpha f ,\quad M_{\alpha\beta}=\int d\mathbf{v}\, v_\alpha v_\beta f , \tag{6}$$

etc. Our primary interest here is in the first of these, $M_0(x,y)=n(x,y)$. The moments satisfy the set of equations obtained from (3) by multiplication and integration, e.g., $\int d\mathbf{v}$, $\int d\mathbf{v}\, v_x$, etc. Since (5) contains five independent functional parameters we will require five independent equations to determine these quantities. The choice of moment equations is not unique and we choose the continuity, x and y momentum, energy, and stress equations. These are found from (3) as described above: continuity,

$$\frac{\partial}{\partial x}M_x+\frac{\partial}{\partial y}M_y=0 , \tag{7}$$

x momentum,

$$\frac{\partial}{\partial x}M_{xx}+\frac{\partial}{\partial y}M_{xy}+\zeta M_x=0 , \tag{8}$$

y momentum,

$$\frac{\partial}{\partial x}M_{xy}+\frac{\partial}{\partial y}M_{yy}+\zeta M_y=0 , \tag{9}$$

energy,

$$\frac{\partial}{\partial x}(M_{xxx}+\alpha M_x)+\frac{\partial}{\partial y}4M_y+2\zeta(M_{xx}-M_0)=0 , \tag{10}$$

stress,

$$\alpha\frac{\partial}{\partial x}M_y+\alpha\frac{\partial}{\partial y}M_x+2\zeta M_{xy}=0 , \tag{11}$$

where $(\alpha/\zeta)=D$, the diffusion coefficient. In writing (7)–(11) we have made use of the following relationships that are a direct result of (5):

$$M_{yy}=\alpha M_0,\quad M_{yyy}=3\alpha M_y,\quad M_{xxy}=\alpha M_y,\quad M_{yyx}=\alpha M_x . \tag{12}$$

The five independent variables may be taken as M_0, M_x, M_y, M_{xx}, and M_{xxx}, which are given directly from (5) as

$$M_0=\tfrac{1}{2}(n_1+n_2)+(2\pi\alpha)^{-1/2}(n_1u_1-n_2u_2)\equiv\tfrac{1}{2}N^{+}+(2\pi\alpha)^{-1/2}J_x^{-} , \tag{13}$$

$$M_x=(\alpha/2\pi)^{1/2}(n_1-n_2)+\tfrac{1}{2}(n_1u_1+n_2u_2)\equiv(\alpha/2\pi)^{1/2}N^{-}+\tfrac{1}{2}J_x^{+} , \tag{14}$$

$$M_y=\tfrac{1}{2}N^{-}w , \tag{15}$$

$$M_{xx}=(\alpha/2)N^{+}+(2\alpha/\pi)^{1/2}J_x^{-} , \tag{16}$$

$$M_{xxx}=\alpha(2\alpha/\pi)^{1/2}N^{-}+(3\alpha/2)J_x^{+} , \tag{17}$$

in terms of which

$$M_{xy}=M_y(3\alpha M_x-M_{xxx})(2\alpha M_0-M_{xx})^{-1} . \tag{18}$$

III. SOLUTION FOR THE CASE OF HIGH FRICTION

The solution to the system (7)–(11) reduces to the consideration of a fourth-order ordinary differential equation (ODE) in (x,q) for which we have been unable to obtain a solution. We therefore consider the case where ζ may be taken as a large quantity so that an expansion of the moments in ζ^{-1} can be considered. We assume that $n(0,y)$ is $O(\zeta^0)$ and that each moment can be expanded as

$$M = M^0 + \zeta^{-1}M^1 + \zeta^{-2}M^2 + \cdots \ . \tag{19}$$

Since the DE follows from the FPE in the high friction limit[11] we expect that the lowest-order solution should reduce to the DE result and that the first nonvanishing higher-order term(s) will contain the information we are seeking. This will be confirmed; however, we will see that in order to determine M_0^1 we will also have to consider some of the M^2 terms as well.

The expansion (19) should be considered as a "bookkeeping" scheme for use with the moment equations; we might not expect to obtain uniformly valid (in x) results from this procedure due to the form of these equations, in which the small parameter $1/\zeta$ multiplies the derivative term. However, as we show, this expansion does not lead to problems with the boundary conditions since the equations themselves satisfy the "extra" boundary conditions resulting from the reduction in order of the differential equation system. In the Appendix we examine a simple model FPE and show that in lowest nonvanishing order the expanded equations have the *identical* solution for the boundary density as is obtained by expanding the exact solution. This result supports our use of the expanded moment equations in what follows.

Expanding the moments according to (19), substituting into (7)–(11), and separating quantities of like order in ζ^{-1}, we find in lowest order:

$$M_x^0 = M_y^0 = M_{xy}^0 = 0 \ , \tag{20a}$$

$$M_{xx}^0 = M_0^0 \ . \tag{20b}$$

Further, (20a) together with (10) implies $M_{xy}^1 = 0$, from which, with (20a) again, it follows that

$$M_{xxx}^0 = 0 \ . \tag{20c}$$

Using (20b) in (7)–(9) we find the following equations in $O(\zeta^0)$:

$$\frac{\partial}{\partial x}M_x^1 + \frac{\partial}{\partial y}M_y^1 = 0 \ , \tag{21a}$$

$$\alpha\frac{\partial}{\partial x}M_0^0 + M_x^1 = 0 \ , \tag{21b}$$

$$\alpha\frac{\partial}{\partial y}M_0^0 + M_y^1 = 0 \ , \tag{21c}$$

so that, eliminating M_x^1 and M_y^1

$$\nabla^2 M_0^0 = 0 \ . \tag{22}$$

Since (20a)–(20c) imply ${}^0N^- = 0$, or $n_1^0 = n_2^0$ (where we use a left superscript to denote the order of terms with a right superscript) then the boundary condition $n_2^0(L,y) = 0$ implies $n_1^0(L,y) = 0$, so that ${}^0N^+(L,y) = 0$. Further, (20c) implies ${}^0J_x^- = 0$, so that from (13) we have

$$M_0^0(L,y) = 0 \tag{23}$$

which together with (22) and the prescribed density at $x = 0$ completely defines the solution in lowest order. As stated earlier, this is identical to the DE solution. As noted above, we only need to specify two boundary conditions (in x) and the equations themselves then ensure that the remaining boundary requirements (in x) are satisfied; this will be seen more clearly below when we consider M_0^1.

To determine M_0^1 we consider those terms in (7)–(11) involving that quantity plus the related equations required for closure:

$$\frac{\partial}{\partial x}M_x^2 + \frac{\partial}{\partial y}M_y^2 = 0 \ , \tag{24a}$$

$$\frac{\partial}{\partial x}M_{xx}^1 + M_x^2 = \alpha\frac{\partial}{\partial x}M_0^1 + M_x^2 = 0 \ , \tag{24b}$$

$$\alpha\frac{\partial}{\partial y}M_0^1 + M_y^2 = 0 \ , \tag{24c}$$

where the final form of (24b) follows from (11) since $M_y^0 = M_x^0 = M_{xxx}^0 = 0$; note that since M_y^i, M_x^i, M_{xxx}^i are not zero for $i \geq 1$ we will not necessarily have

$$\alpha M_0^{i+1} = M_{xx}^{i+1} \ .$$

Comparing (21) and (24) we see that

$$\nabla^2 M_0^1 = 0 \ . \tag{25}$$

This is to be solved subject to the boundary conditions

$$n_2^1(L,y) = M_0^1(0,y) = 0 \ . \tag{26}$$

The latter has been arbitrarily chosen since we have the freedom to specify the density at $x = 0$. To find $n_2^1 = ({}^1N^+ - {}^1N^-)/2$ we use (13)–(18), for which purpose we also need M_x^1, M_y^1, M_{xxx}^1. The first two of these follow from (21b) and (21c) together with the known result for M_0^0. The latter is then found from (18) after solving (10) for M_{xy}^2 using M_x^1, M_y^1. We find

$$\overline{M}{}_{xy}^2 = \alpha^2 i q^2 \bar{n}(0,q)\left[\frac{e^{-qx} + e^{-q(2L-x)}}{1 - e^{-2qL}}\right] \ , \tag{27}$$

$$M_{xxx}^1 = 2\alpha M_x^1 \ . \tag{28}$$

The consequences of (28) together with the extension of (20b) to $O(1/\zeta)$ are that ${}^1J_x^- = {}^1J_x^+ = 0$ everywhere, so that the missing boundary condition for the emergent flux at the absorbing boundary is satisfied and we are able to determine the two constants which appear in the solution of (25) using only (26) without violating the flux condition. From (13) and (14) we have

$$n_2^1 = M_0^1 - (\pi/2\alpha)^{1/2} M_x^1 \ , \tag{29}$$

which together with the result found earlier for M_x^1 leads directly to the solution of the system (25), (26) that determines $\overline{M}{}_0^1$:

$$\overline{M}{}_0^1(x,q) = (2\pi\alpha)^{1/2}\frac{\bar{n}(0,q)qe^{-2qL}}{(1 - e^{-2qL})^2}(e^{qx} - e^{-qx}) \ . \tag{30}$$

IV. DISCUSSION

The above result is no more tractable than the classical result (2) and for this reason we will confine our attention here to the boundary solution:

$$\overline{M}\,_0^1(L,q)=(2\pi\alpha)^{1/2}\frac{\bar{n}(0,q)q}{\sinh(qL)}\ , \tag{31}$$

which can be written in the physical space as

$$M_0^1(L,y)=(\alpha/2\pi)^{1/2}(\pi/2L)^2 \times \int dy'\frac{n(0,y')}{\cosh^2[(y-y')\pi/2L]}\ . \tag{32}$$

If $n(0,y)$ is concentrated at a single point we see that this will be mirrored on the boundary. However, if $n(0,y)$ is concentrated at two (or more) points this will not be directly mirrored on the boundary. For the latter case we consider

$$n(0,y)=\frac{n_0}{2}[\delta(y-a)+\delta(y+b)]\ ,$$

with $0<a<b\ll 2l/\pi$ and easily find, e.g.,

$$M_0^1(L,0)>1+[\cosh^2(a+b)\pi/2L]^{-1}>M_0^1(L,a) =M_0^1(L,-b)\ .$$

This result indicates that preferential accumulation may occur on the boundary and that the points (or regions) where this occurs do not directly mirror the known distribution at $x=0$.

The validity of our results rest on the creditability of the high friction coefficient expansion introduced through (19). As we have indicated, the lost boundary condition problem is not an issue here as the equations ensure that the necessary conditions are satisfied. Note especially that (21b) and (21c), and (24b) and (24c), ensure that Fick's law holds through $0(1/\zeta^2)$. This is very much like the situation encountered with the Chapman-Enskog solution of the Boltzmann equation,[12,13] where a similar ordering of streaming and collisional terms is used. In the Appendix we consider a model FPE, obtain the exact solution for the 2D absorbing boundary problem considered above, and show that the expanded solution is identical to the result obtained from the expanded equations. Thus our treatment appears to be well motivated and further investigations of the boundary behavior demonstrated above using more sophisticated techniques should be warranted.

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APPENDIX

We consider a generalization of the Goldstein model[14,15] to two dimensions: the four allowable particle velocities are[16]

$$\mathbf{v}=(v_x,v_y)=(1,0),(0,-1),(-1,0),(0,1) =v_1,v_2,v_3,v_4$$

so that if the distribution function for v_i is denoted as n_i we have

$$\frac{\partial}{\partial x}n_1=\frac{\gamma}{4}(n_2+n_3+n_4-3n_1)\ , \tag{A1}$$

$$-\frac{\partial}{\partial y}n_2=\frac{\gamma}{4}(n_1+n_3+n_4-3n_2)\ , \tag{A2}$$

$$-\frac{\partial}{\partial x}n_3=\frac{\gamma}{4}(n_1+n_2+n_4-3n_3)\ , \tag{A3}$$

$$\frac{\partial}{\partial y}n_4=\frac{\gamma}{4}(n_1+n_2+n_4-3n_4)\ . \tag{A4}$$

Here γ plays the role of the friction coefficient. Solving these equations for $\overline{N}(x,q)=\sum_i\bar{n}_i(x,q)$ subject to the boundary condition that $N(0,y)$ is given and the emergent density at $x=L$ vanishes, $n_3(L,y)=0$, we find that the boundary density $\overline{N}(L,q)$ is

$$\overline{N}(L,q)=\frac{\overline{N}(0,q)2a\gamma^{-1}}{\sinh(aL)+a\gamma^{-1}\cosh(La)}\ , \tag{A5}$$

where $a=[q^2(1+2q^2\gamma^{-2})^{-1}]^{1/2}$. Expanding this for small γ^{-1} we find

$$\overline{N}(L,q)=\overline{N}\,^0(L,q)+\gamma^{-1}\overline{N}\,^1(L,q)+\cdots\ ,$$

with

$$\overline{N}\,^0=0,\quad \overline{N}\,^1=2q\overline{N}(0,q)/\sinh(qL)\ .$$

The latter result, except for a model-dependent constant prefactor, is identical to the main result of our paper, (31), and is identical to the result obtained by direct expansion of (A1)–(A4). Our previous result thus also applies to the expansion of the exact solution for this model.

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