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2D Brownian motion in a system of reflecting barriers: effective diffusivity by a sampling method

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Abstract. We study two-dimensional Brownian motion in an ordered periodic system of linear reflecting barriers using the sampling method and conformal transformations. We calculate the effective diffusivity for the Brownian particle. When the periods are fixed but the length of the barrier goes to zero, the effective diffusivity in the direction perpendicular to the barriers differs from the standard one by a term of order ϵ^2 where ϵ is the length of a barrier.

1. Introduction

Brownian motion in the presence of absorbing traps is a problem related to various physical phenomena, e.g. diffusion limited reaction [1–3], diffusion limited aggregation [4, 5], fluids in porous media [6, 7] and diffusion of photons in a random or turbid media [8]. In general the study of the Brownian motion in systems with either absorbing or reflecting barriers (or the combination of both) has great potential applications in various disciplines such as biology, chemistry or physics [9]. In many disordered systems the transport properties are closely related to that of the Brownian motion. Recently we have studied the problem of the Brownian motion in a periodic system of absorbing traps [10].

Brownian motion in a system of periodic reflecting obstacles has been extensively studied, see e.g. a classic book [11]; see [12] for some of the most recent developments. It is known that, on the large scale, the process behaves like the ordinary Brownian motion with different diffusion coefficients. However, no explicit formulae for effective diffusivity can be given except in trivial cases. One can approach the problem using partial differential equations [21]. We will show how the methods developed in [10] can be applied to calculate effective diffusivity in a special non-trivial case. We will also derive an asymptotic formula for the effective diffusivity when the length of reflecting line segments goes to zero.

We will consider a two-dimensional (2D) Brownian motion in a system of linear reflecting barriers, as shown in figure 1. The system is periodic in the x-direction with period $A + B$. The size of the gate between the barriers on a line is A and the size of a barrier is B. The distance between the lines is $\pi/2$ and this sets the length scale in the system. Unlike in the previous case [10], here we do not demand periodicity in the y-direction. Instead, the second period is given by a vector $(C, \pi/2)$. Whenever a Brownian trajectory hits a black line (barrier) it is reflected with the normal vector of reflection (for the discussion and applications of reflected Brownian motion with oblique angle of reflection see e.g. [13]). In order to find the effective diffusivity we will employ the conformal invariance of Brownian motion [14], i.e. the invariance of Brownian motion under local

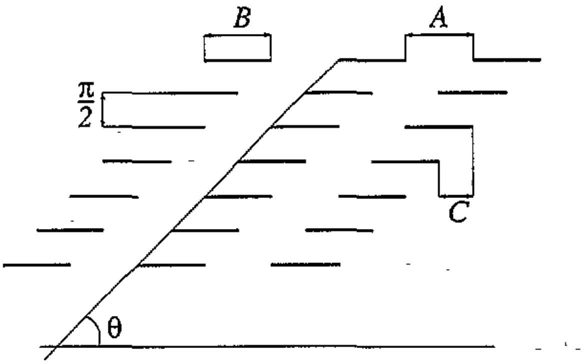

Figure 1. The system of reflecting barriers with period $A + B$ along the x-axis and shift C between the lines. The size of the gate is A and the distance between two neighbouring lines of gates is $\pi/2$. θ is the inclination of the channel formed by the gates ($\tan\theta = \pi/2C$).

rotations and local changes of spatial and temporal scale, and the sampling method for the Brownian motion [15, p 413].

The conformal invariance property has been a working tool in the case of 2D critical systems [16] and in 2D polymer systems modelled as self-avoiding random walks [17]. In the case of 2D critical systems, conformal invariance is a symmetry of the critical system which gives powerful information on the dynamics (critical exponents). In this work conformal invariance is used as a purely technical tool.

The sampling method corresponds to the detection of the Brownian particle in some prescribed regions in space. It is used to compute averages over the ensemble of Brownian trajectories. We will use a technique known as the 'optional sampling theorem' [15, p 438].

Before we proceed, let us consider a simple case which provides us with a quick insight into the problem. Let $Z(t) = (Z_1(t), Z_2(t))$ be the location of the reflecting Brownian particle after time t. The distribution of $Z(t)/\sqrt{t}$ approaches a Gaussian distribution ρ for large t [11]. Let $R = (X, Y)$ have ρ distribution. This distribution is characterized by only three cumulants [9]: $\langle X^2\rangle$, $\langle Y^2\rangle$ and $\langle XY\rangle$ because $\langle X\rangle = \langle Y\rangle = 0$ due to the symmetry. At this point we shall consider a simple limit. In the case when the size of the barriers approaches zero we find by symmetry the following standard result:

$$\rho(x, y) = \frac{1}{2\pi}\exp\left(-x^2/2 - y^2/2\right). \tag{1.1}$$

For convenience the diffusion constant has been set to 1 throughout the paper. The level curves in this case (the probability density ρ is the same at each point of such a curve) are circles and the motions along the x- and y-axes are uncorrelated, i.e. $\langle XY\rangle = 0$. The averages over the ensemble of Brownian trajectories will be denoted $\langle\cdots\rangle_B$, while $\langle\cdots\rangle$ will be the average obtained from the asymptotic distribution.

We note that in every system of reflecting barriers parallel to the x-axis, the barriers do not disturb the motion along them (i.e. in the x-direction) thus the distribution along x is the same as for the system with no barriers (1.1) and so $\langle X^2\rangle = 1$.

Consider the case when neither gates nor traps have zero length. The reflecting barriers have a damping effect on the motion in every direction which is not parallel to the x-axis. In other words, $\langle(X\cos\theta + Y\sin\theta)^2\rangle < 1$ for every angle $\theta \in (0, \pi)$. Since $\langle X^2\rangle = 1$, the level curve of ρ must be an ellipse whose long axis is parallel to the x axis. Hence, the distribution for the system of reflecting barriers is given by the following formula:

$$\rho(x, y) = \frac{1}{2\pi\sqrt{\langle Y^2\rangle}} \exp\left(-x^2/2 - y^2/2\langle Y^2\rangle\right). \tag{1.2}$$

We see that $\langle XY\rangle = 0$ in all cases. As could be expected $\langle Y^2\rangle \leqslant 1$. In the rest of this paper we compute $\langle Y^2\rangle$ using the conformal transformations and the sampling method. From now on we shall assume that we have reached the asymptotic limit, so all our calculations hold for large times only.

The paper is arranged as follows. In section 2 we present our sampling method which is used to calculate the aforementioned averages. In section 3 we use conformal transformations to obtain the density of the hitting (probability) distribution [10] (or in other words the transition probabilities [9], or density of harmonic measure [15, p 13; 18]) in our scheme. In section 4, we present the formulae for the averages using the sampling method described in the previous sections. In section 5 we give an explicit asymptotic formula for $\langle Y^2\rangle$ in the case of vanishing barrier size. The numerical results and the discussion are presented in section 5. Some of our calculations have been relegated to appendices.

2. Sampling of the Brownian motion

The sampling method corresponds to detection of the Brownian motion only at selected points in space. The particle will move through the gates. Once it starts from a gate on a given line we set our 'detectors' on the neighbouring lines. The particle starting at time $T(0)$ reaches a neighbouring line at time $T(1)$. It can either enter a gate or hit a barrier. If it hits a gate we set our 'detectors' on the lines below and above the gate. It may also reach the upper line and hit a barrier from below, or reach the lower line and hit a barrier from above. Suppose it hits a barrier on the line above. Once it does so we set our detectors on the same line and on the line below. If it hits a barrier on the line below we set the detectors on the same line and the line above. We continue this procedure using three starting schemes: from the gate, from below the barrier and from above the barrier, and monitor the points where the particle hits the lines according to the aforementioned scheme. The consecutive times when the Brownian particle is observed will be called $T(0), T(1), T(2)$, etc. Other sampling schemes are possible and some of them are much simpler but they do not seem to be amenable to numerical calculations.

For each step in our sampling scheme we introduce a transition vector

$$\boldsymbol{V}(k) = \boldsymbol{Z}(T(k)) - \boldsymbol{Z}(T(k-1)) \tag{2.1}$$

for the transition between the moments $T(k-1)$ and $T(k)$ of detection of the kth step. By a version of the central limit theorem for dependent random variables [19] the distribution of the random variable

$$\sum_{k=1}^{m} \frac{\boldsymbol{V}(k)}{\sqrt{m}} \tag{2.2}$$

approaches, for large m, a Gaussian distribution. Let $\boldsymbol{W} = (W_1, W_2)$ have this limiting distribution. Then $\boldsymbol{W}/\bar{t} = \boldsymbol{R}$ in the sense of equality of distributions (see previous section for the definition of $\boldsymbol{R}$). Here $\bar{t}$ is the expected value of the duration of the single step in our sampling method. The relation between $\boldsymbol{W}$ and $\boldsymbol{R}$ is easy to understand if we note that $T(m) = m\bar{t} + O(\sqrt{m})$. We also have

$$\langle W_i W_i \rangle = \lim_{m\to\infty} \sum_{k=1}^{m} \sum_{l=1}^{m} \frac{1}{m} \langle V_i(k) V_i(l) \rangle_{\mathrm{B}} \tag{2.3}$$

for $i = 1, 2$. We will assume that the initial distribution of the process is uniform on a fixed line. Then the process is in the stationary regime and we have $\langle V_i(k) V_i(k+l) \rangle_{\mathrm{B}} = \langle V_i(1) V_i(1+l) \rangle_{\mathrm{B}}$ for every k and $l \geqslant 0$. The covariance $\langle V_i(k) V_i(k+l) \rangle_{\mathrm{B}}$ goes to zero exponentially fast as l goes to infinity. These two facts and an easy calculation show that (2.3) may be simplified as follows:

$$\langle W_i W_i \rangle = \langle V_i^2(1) \rangle_{\mathrm{B}} + 2 \sum_{k=2}^{\infty} \langle V_i(1) V_i(k) \rangle_{\mathrm{B}} \,. \tag{2.4}$$

One can also express the cumulants of $\boldsymbol{R} = (X, Y)$ in terms of those of $\boldsymbol{W} = (W_1, W_2)$ by noting that $\langle X^2 \rangle = 1$. In particular we have

$$\langle Y^2 \rangle = \frac{\langle W_2^2 \rangle}{\langle W_1^2 \rangle} \,. \tag{2.5}$$

Before we can calculate the ensemble averages $(\langle \cdots \rangle_{\mathrm{B}})$ in (2.4) we have to specify the transition probabilities between successive steps. It is done in the next section. Additionally we note that the time variable will not enter into the calculations.

3. Transition probabilities

According to our sampling scheme we have two general situations: start at the time $T(k-1)$ from a gate or start from a barrier (the cases of the start from above and below a barrier are symmetric). The 'detectors' are on two lines at a time. In both cases we have to compute transition probabilities of reaching these lines. These two different situations are shown schematically in figures 2(*a*) and 2(*b*).

The case when we start from a gate corresponds to a stripe of width π where the starting point is in the middle of the stripe and the particle may be reflected by barriers in the middle of the stripe. This situation is equivalent to a stripe of the same width with no reflecting barriers in the middle. The reason is that the hitting place on the upper or lower line depends on the place where the particle leaves the middle line for the last time but this place is not affected by the presence of the barriers.

In the case of the start from above a barrier the 'detectors' are placed on the line above and on the same line, except that there are no detectors on the barrier from which the particle starts. By using reflection, this situation is equivalent to a stripe of width π with two half-lines in the middle and a single gate between the half-lines (figure 2(*b*)). In this case, the length of the gate is equal to B, i.e. it is the same as the length of the barrier in the original stripe. The hitting probabilities in the new stripe correspond to those in the original stripe of width $\pi/2$ by symmetry with respect to the middle line. One has to multiply the probabilities by 2 or, in other words, sum the probabilities of hitting the points in the upper and lower part of the stripe in order to obtain the probabilities in the original stripe.

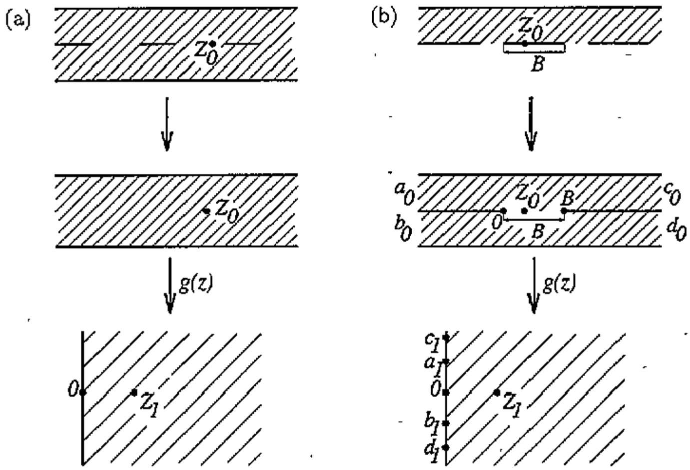

Figure 2. (*a*) The domain used to calculate the one-step transition probabilities for the particle starting from a point z_0 in a gate. The reflecting barriers in the middle of the stripe can be removed. The probabilities of hitting 'detectors' on solid lines are not changed. Here $g(z) = \exp(z)$ and $z_1 = \exp(z_0)$. (*b*) The domain used to calculate the one-step transition probabilities for the particle starting from a point z above a barrier. The probabilities are the same as for the particle starting from a gate of length B in a stripe of double width with two half-lines removed. The 'detectors' are placed on both solid lines and both sides of each half-line in the transformed domain. Here $g(z) = \sqrt{(\exp(2z) - 1)/(\exp(2B) - \exp(2z))}$, $z_1 = \sqrt{(\exp(2z_0) - 1)/(\exp(2B) - \exp(2z_0))}$, $g(a_0) = a_1 = \mathrm{i}\mathrm{e}^{-B}$, $g(b_0) = b_1 = -\mathrm{i}\mathrm{e}^{-B}$, $g(c_0) = c_1 = \mathrm{i}$, $g(d_0) = d_1 = -\mathrm{i}$, $g(0) = 0$, $g(B) = 0 \cdot \mathrm{i} + \infty$.

In order to find transition probabilities we use conformal transformations. From now on we shall use complex variables z. Let $h(z, z')\mathrm{d}z'$ denote the probability that the particle starting at point z will reach the point $z' \pm \mathrm{d}z'/2$. This probability is easy to find for the half-plane bounded by the imaginary axis. We have, in this case, the Cauchy distribution [20]

$$h_0(z, z') = \frac{\mathrm{Re}(z)}{\pi |z - z'|^2} \tag{3.1}$$

where z is any point in the right half-plane and z' lies on the imaginary axis. Now we can transform the stripes shown in figures 2(*a*),(*b*) onto the half-plane and the probabilities will transform according to the following formula:

$$h(z, z') = h_0(g(z), g(z')) \left| \frac{\mathrm{d}g(z')}{\mathrm{d}z'} \right| \tag{3.2}$$

where h, h_0 are the transition probabilities for the stripe and half-plane, respectively, and g is a one-to-one mapping of the stripe onto the half plane. In the situation shown in figure 2(*a*)

$$g(z) = \exp(z) \tag{3.3}$$

while for the figure 2(*b*) we have

$$g(z) = \sqrt{\frac{\exp(2z) - 1}{\exp(2B) - \exp(2z)}}. \tag{3.4}$$

In both cases the mapping is onto $H = \{z : \mathrm{Re}(z) > 0\}$. The detailed discussion of these calculations has been relegated to appendix A.

4. The sampling averages

In this section we shall give the formulae for the average $\langle V_i(1)V_i(k)\rangle_B$ which appear in (2.4). Once we have these averages the computation of $\langle Y^2\rangle$ (see (1.2)) is straightforward as discussed in section 2.

First of all we introduce a new variable, $\hat{x}$

$$\hat{x} = (x, n\pi/2; \beta) \tag{4.1}$$

where x denotes the x-coordinate and $n\pi/2$ gives the y-coordinate (n is an integer). If x is in a gate then $\beta = 0$, if x is just below a barrier then $\beta = -1$ and if it is just above a barrier then $\beta = 1$. Thus β describes three different starting positions for a step in our sampling scheme. Let $P_2(\hat{x}_{k-1}, \hat{x}_k)$ be the transition probability for the kth step. It is easy to see that P_2 vanishes unless one of the following conditions is satisfied:

(1) $\beta_{k-1} = 0$ and $n_k - n_{k-1} = -1, +1$;
(2) $\beta_{k-1} = +1$ and $n_k - n_{k-1} = +1, 0$;
(3) $\beta_{k-1} = -1$ and $n_k - n_{k-1} = -1, 0$.

Moreover, $P_2(\hat{x}_{k-1}, \hat{x}_k)$ vanishes when:

(i) $\beta_{k-1} = +1$, $\beta_k = +1$ and $n_k - n_{k-1} = +1$;
(ii) $\beta_{k-1} = +1$, $\beta_k = -1$ and $n_k - n_{k-1} = 0$;
(iii) $\beta_{k-1} = -1$, $\beta_k = -1$ and $n_k - n_{k-1} = -1$;
(iv) $\beta_{k-1} = -1$, $\beta_k = +1$ and $n_k - n_{k-1} = 0$.

P_2 is directly related to transition probabilities discussed in section 3 and appendix A. For example, suppose that $\hat{x}_{k-1} = (x_{k-1}, n_{k-1}\pi/2; 0)$ and $\hat{x}_k = (x_k, (n_{k-1}+1)\pi/2; -1)$. Then (A.2) yields

$$\begin{aligned} P_2(\hat{x}_{k-1}, \hat{x}_k)\mathrm{d}x_k &= p(x_{k-1}; x_k - \mathrm{d}x_k/2, x_k + \mathrm{d}x_k/2) \\ &= \frac{1}{\pi}(\arctan(\exp(x_k + \mathrm{d}x_k/2)/\exp(x_{k-1})) \\ &\quad - \arctan(\exp(x_k - \mathrm{d}x_k/2)/\exp(x_{k-1}))) \,. \end{aligned} \tag{4.2}$$

Now we can write the average $\langle V_1(1)V_1(k)\rangle_B$ in the following form [9]:

$$\begin{aligned} \langle V_1(1)V_1(k)\rangle_B = \sum_{n_0,\beta_0}\cdots\sum_{n_k,\beta_k}\int \mathrm{d}x_0 P_1(\hat{x}_0)\int \mathrm{d}x_1(x_1 - x_0)P_2(\hat{x}_0, \hat{x}_1) \\ \times \int \mathrm{d}x_2 P_2(\hat{x}_1, \hat{x}_2)\cdots\int \mathrm{d}x_k(x_k - x_{k-1})P_2(\hat{x}_{k-1}, \hat{x}_k) \end{aligned} \tag{4.3}$$

where P_1 is the initial distribution for P_2. A similar formula holds for $\langle V_2(1)V_2(k)\rangle_B$:

$$\begin{aligned} \langle V_2(1)V_2(k)\rangle_B = \sum_{n_0,\beta_0}\cdots\sum_{n_k,\beta_k}\int \mathrm{d}x_0 P_1(\hat{x}_0)\int \mathrm{d}x_1((n_1 - n_0)\pi/2)P_2(\hat{x}_0, \hat{x}_1) \\ \times \int \mathrm{d}x_2 P_2(\hat{x}_1, \hat{x}_2)\cdots\int \mathrm{d}x_k((n_k - n_{k-1})\pi/2)P_2(\hat{x}_{k-1}, \hat{x}_k) \,. \end{aligned} \tag{4.4}$$

In order to simplify calculations we introduce a new transition probability, $Q(\hat{x}, \hat{z})$,

$$Q(\hat{x}, \hat{z}) = \sum_{m,n} P_2(\hat{x}, \hat{y}) \tag{4.5}$$

where $\hat{x} = (x, 0; \beta)$, $\hat{z} = (z, 0; \beta')$, $\hat{y} = (m(A+B)+Cn+z, n\pi/2; \beta')$, $0 < x, z < A+B$, and $n = 0, \pm 1$. The new transition probability enables us to deal with the interval $(0, A+B)$ rather than the whole real line and thus considerably shortens the numerical calculations. Q may be interpreted as the transition probability in the case when we specify the distance of the hitting point from the left endpoint of the gate (we choose the closest one which lies to the left of the hitting point) but otherwise we ignore the position of the hitting point. This is possible since the system of barriers is doubly periodic.

Let $\tilde{x}$ be chosen so that $\hat{x} - \tilde{x}$ belongs to $\{y = 0, 0 < x < A + B\}$. Now Q acts in the single gate and barrier and (4.3) can be rewritten in the following form amenable for numerical calculations:

$$\langle V_1(1)V_1(k)\rangle_B = \sum_{\beta_0}\sum_{n_1,\beta_1}\sum_{\beta_2}\cdots\sum_{\beta_{k-1}}\sum_{n_k,\beta_k}\int_{A_{\beta_0}} dx_0\alpha(\hat{x}_0)\int dx_1(x_1 - x_0)P_2(\hat{x}_0, \hat{x}_1)$$
$$\times\int_{A_{\beta_2}} dx_2 Q(\hat{x}_1 - \tilde{x}_1, \hat{x}_2)\int_{A_{\beta_3}} dx_3 Q(\hat{x}_2, \hat{x}_3)\cdots\int dx_k(x_k - x_{k-1})P_2(\hat{x}_{k-1}, \hat{x}_k) \tag{4.6}$$

where α is the stationary distribution for Q, i.e.

$$\alpha(\hat{x}) = \int_{A_\beta} dy Q(\hat{y}, \hat{x})\alpha(\hat{y}) \qquad \hat{y} = (y, 0; \beta). \tag{4.7}$$

Here the intervals A_β are as follows: $A_0 = \{x : 0 < x < A\}$ and $A_1 = A_{-1} = \{x : A < x < A + B\}$. Equation (4.4) may be expressed in a form analogous to (4.6). These equations are used in the next section to compute the averages numerically. Note that the integration over the whole real line involving P_2 appears only twice in (4.6). The calculations which lead to (4.6) are contained in appendix B.

5. Asymptotic formula in the case of small barriers

We will show that when the barrier length $B = \epsilon$ approaches zero and the period $A + \epsilon$ is kept constant then

$$\langle Y^2\rangle(\epsilon) = 1 - \epsilon^2/(2A) + o(\epsilon^2). \tag{5.1}$$

Note that the shift C does not appear in this formula. The above formula might have some interest as it is related to the following conjecture. Fix some planar set F with non-zero area. Place a copy ϵF of the set F rescaled by ϵ at each vertex of the standard two-dimensional lattice and let Z' be a Brownian motion reflected from these obstacles. It has been conjectured that the effective diffusivity of Z' should be equal to

$$1 - c\epsilon^2\text{Area}(F) \tag{5.2}$$

where c is an absolute constant, i.e. it does not depend on the shape of F. Note that we obtain the correction of order ϵ^2 in (5.1) despite the fact that line segments have zero area.

In order to find an asymptotic formula for the effective diffusivity when the size of the barriers goes to zero we change our sampling scheme. The position of the particle will be detected whenever it reaches a neighbouring line. The sequence of times when this happens will be denoted $S(0), S(1), S(2)$, etc. We will assume that the process starts at time $S(0) = 0$ with the initial distribution uniform on a line. The transition vector for the step between times $S(k-1)$ and $S(k)$ will be denoted $U(k)$, i.e.

$$U(k) = Z(S(k)) - Z(S(k-1)). \tag{5.3}$$

Recall that the size of a barrier will be denoted ϵ rather than B. We will suppose that the period $A + \epsilon$ is fixed and ϵ approaches zero. Recall that

$$\sum_{k=1}^{m} \frac{U(k)}{\sqrt{m}} \tag{5.4}$$

converges to a Gaussian variable, say $M = (M_1, M_2)$. We have

$$\langle M_2 M_2 \rangle = \langle U_2^2(1) \rangle_{\mathrm{B}} + 2\sum_{k=2}^{\infty} \langle U_2(1) U_2(k) \rangle_{\mathrm{B}}. \tag{5.5}$$

Observe that the expected value $\bar{s}$ of $S(k) - S(k-1)$ does not depend on the size or position of the barriers as long as they are confined to horizontal lines $\pi/2$ units apart. Hence

$$\langle Y^2 \rangle(\epsilon) = \frac{\langle Y^2 \rangle(\epsilon)}{\langle Y^2 \rangle(0)} = \frac{\langle M_2 M_2 \rangle(\epsilon)}{\langle M_2 M_2 \rangle(0)} \tag{5.6}$$

where the dependence on the parameter ϵ is made explicit in the notation. Note that we always have $U_2(k) = \pm\pi/2$. When there are no barriers, i.e. when $\epsilon = 0$, then the steps $U(k)$ are uncorrelated and we obtain, from (5.5),

$$\langle M_2 M_2 \rangle(0) = \langle U_2^2(1) \rangle_{\mathrm{B}} = \pi^2/4. \tag{5.7}$$

Now suppose that $\epsilon > 0$. If $Z(S(1))$ is in the gate then the next step may be positive or negative with the same probability and $U_2(1)$ and $U_2(2)$ are uncorrelated. Suppose that $Z(S(1))$ is just below a barrier. This means that the first step was upward, i.e. $U_2(1) - U_2(0) = \pi/2$. The steps $U_2(1)$ and $U_2(2)$ will not be correlated if the Brownian particle hits a gate on the line containing $Z(S(1))$ before hitting the line containing $Z(S(0))$ because in this case the next step, $U_2(2)$, between $S(1)$ and $S(2)$ may be positive or negative with the same probability. It remains to consider the case when $Z(S(1))$ is just below a barrier and the process starting from $Z(S(1))$ hits the line containing $Z(S(0))$ before hitting any part of the line containing $Z(S(1))$. In this case, the steps will be negatively correlated. It will be shown in appendix C that the probability of such an occurrence is equal to $\epsilon/4 + \mathrm{o}(\epsilon)$. The probability that $Z(S(1))$ belongs to a barrier is equal to $\epsilon/A + o(\epsilon)$ for small ϵ. The cases when $Z(S(1))$ is just below a barrier and just above a barrier are symmetric. Hence

$$\langle U_2(1) U_2(2) \rangle_{\mathrm{B}} = -(\epsilon/4 + \mathrm{o}(\epsilon))(\epsilon/A + \mathrm{o}(\epsilon))(\pi^2/4) = -(\pi^2/4)(\epsilon^2/(4A) + \mathrm{o}(\epsilon^2)). \tag{5.8}$$

The terms $\langle U_2(1) U_2(k) \rangle_{\mathrm{B}}$ with $k > 2$ are of order smaller than ϵ^2. We will discuss only $\langle U_2(1) U_2(3) \rangle_{\mathrm{B}}$. Suppose that the process is in the stationary distribution. Then the distribution of $Z(S(1))$ is uniform on a line. If $Z(S(1))$ belongs to a gate then $U_2(1)$ may be positive or negative with the same probability and $U_2(1)$ and $U_2(3)$ are uncorrelated. The same argument applies when $Z(S(2))$ belongs to a gate. The only contribution to

$\langle U_2(1)U_2(3)\rangle_B$ comes from the situation when both $Z(S(1))$ and $Z(S(2))$ lie on barriers and, moreover, the process starting from $Z(S(2))$ hits the line containing $Z(S(1))$ before hitting any part of the line containing $Z(S(2))$. The probabilities of these three events are $\epsilon/A + o(\epsilon)$, $\epsilon/A + o(\epsilon)$ and $\epsilon/4 + o(\epsilon)$. Hence

$$\langle U_2(1)U_2(3)\rangle_B = -(\pi^2/4)(\epsilon^3/(4A^2) + o(\epsilon^3)). \tag{5.9}$$

It follows from (5.5) and (5.8)–(5.9) that

$$\langle M_2 M_2\rangle = (\pi^2/4)(1 - 2\epsilon^2/(4A) + o(\epsilon^2)). \tag{5.10}$$

Thus, (5.6) and (5.7) imply

$$\langle Y^2\rangle(\epsilon) = \frac{(\pi^2/4)(1-\epsilon^2/(2A) + o(\epsilon^2))}{\pi^2/4} = 1 - \epsilon^2/(2A) + o(\epsilon^2). \tag{5.11}$$

6. Numerical results and discussion

In order to perform numerical calculations we have discretized the problem. The period $A+B$ has been divided into 80 small intervals. The hitting probabilities between points have been replaced by the hitting probabilities of a small interval for the process starting from the middle of another interval (see appendix A). The transition probabilities for a single step have been calculated using formulae given in appendix A. They also provide probabilities P_2 as explained in section 4. The modified probabilities Q have been calculated using (4.5). Equation (4.7) becomes a system of linear equations in the discrete case. The system has a unique solution provided we normalize α by $\sum_{\beta}\int_{A_\beta}\alpha(\hat{x})\mathrm{d}x = 1$. Given α, Q and P_2, we have used (4.6) and an analogous formula for $\langle V_2(1)V_2(k)\rangle_B$, (2.4) and (2.5) to find $\langle Y^2\rangle$.

We have done numerical calculations for several sets of parameters A, B and C. The available amount of computer memory enabled us to consider periods $A+B$ ranging between 2 and 16. The barrier size B varied between 1/40 of period $A+B$ and 39/40 of the period. We considered shifts C between 0 and 1/2 of period $A+B$. The results for other shifts may be obtained from ours by using translation invariance and/or symmetry.

First let us discuss the case when A and B are fixed. The influence of the shift C on $\langle Y^2\rangle$ is illustrated in figure 3. In some cases $\langle Y^2\rangle$ is a monotone function of C, for example, when $A = 3.80$, $B = 0.20$ and C varies on the interval (0, 2). In figure 3(*a*) we have $A = 8$ and $B = 2$. The effective diffusivity $\langle Y^2\rangle$ attains its minimum for a value $C = 2.75 \pm 0.125$ and it is not a monotone function of C between 0 and one half of the period.

The behaviour of $\langle Y^2\rangle$ as a function of shift C may be even more complicated as illustrated by figure 3(*b*). Here $A = 14$ and $B = 2$. The graph has two local minima at $C = 2.8 \pm 0.2$ and $C = 6.4 \pm 0.2$ on the interval (0, 8). The lack of monotonicity in the last two cases illustrates the fact that the influence of reflecting obstacles on effective diffusivity is not additive. The increase or reduction of effective diffusivity is in part due to the 'interaction' between the obstacles. When A is large, the interaction between obstacles which are separated by two or more stripes may become important. This effect strongly depends on the configuration and may both increase or decrease as C increases. One may speculate that the graphs of $\langle Y^2\rangle$ as a function of shift C have even more local minima

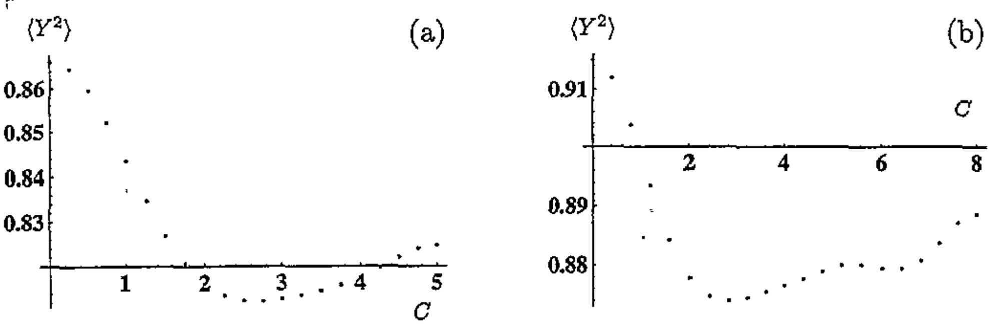

Figure 3. Effective diffusivity $\langle Y^2 \rangle$ as a function of shift C. In (a), period $A + B = 10$, barrier $B = 2$, shift C is increasing from 0 to $(A + B)/2 = 5$. In (b), period $A + B = 16$, barrier $B = 2$, shift C is increasing from 0 to $(A + B)/2 = 8$.

as the gate size grows and the barrier size is kept constant. Limitations on the computer memory prevented us from checking this conjecture.

The asymptotic formula derived in section 5 shows that the influence of shift on effective diffusivity $\langle Y^2 \rangle$ should diminish as the size of the barrier goes to zero. This is strongly supported by the results obtained for parameters mentioned above. Let $\langle Y^2 \rangle^{max}$ and $\langle Y^2 \rangle^{min}$ denote the maximal and minimal value of $\langle Y^2 \rangle$ for the given set of parameters. Let

$$\gamma = \frac{\langle Y^2 \rangle^{\max} - \langle Y^2 \rangle^{\min}}{1 - \langle Y^2 \rangle^{\min}}. \tag{6.1}$$

The value of γ is 0.0044 when $A = 3.80$ and $B = 0.20$, $\gamma = 0.29$ if $A = 8$ and $B = 2$, and $\gamma = 0.33$ for $A = 14$ and $B = 2$.

We present the comparison of the asymptotic formula (5.1) with the results of numerical calculations in figure 4. First we show the results for $A + B = 4$, $C = 0$ and $B = \epsilon$ changing from 0.30 to 2 in increments of 0.10 (see figure 4(a)). Formula (5.1) says that the correction to standard effective diffusivity is equal to $\epsilon^2/(2A)$. We calculated the relative error χ of this correction as compared to the value of $1 - \langle Y^2 \rangle$ obtained numerically,

$$\chi = \frac{\epsilon^2/(2A) - (1 - \langle Y^2 \rangle)}{1 - \langle Y^2 \rangle}. \tag{6.2}$$

The relative error χ decreases as ϵ goes to zero (see figure 4(b)). For ϵ around 0.30, the absolute value of the error χ starts increasing as the size of the subdivision used for numerical integration becomes comparable to the size of the barrier. We find reasonably good agreement of theoretical predictions and numerical results.

Let us summarize our results. We have studied an asymptotic distribution for a two-dimensional Brownian particle in a periodic system of reflecting barriers. The motions along the barriers and perpendicular to the barriers are uncorrelated. The diffusion constant in the direction parallel to barriers remains unchanged while the one perpendicular to barriers is reduced in comparison to the motion in free space. For finite size of the barriers the diffusion constant (perpendicular to barriers) is in general a non-monotonic function of $\tan\theta$, where θ gives the inclination of the channel formed by the barriers (figure 1). In the limit of vanishing barrier size, $B = \epsilon$, fixed period, $A + B$, and fixed distance $\pi/2$ between the lines of barriers it is given by $(1 - \epsilon^2/2A)\sqrt{t}$ (t is time) and does not depend on θ. We hope that the sampling method and conformal transformation method described in this paper will be useful for future studies of the Brownian motion.

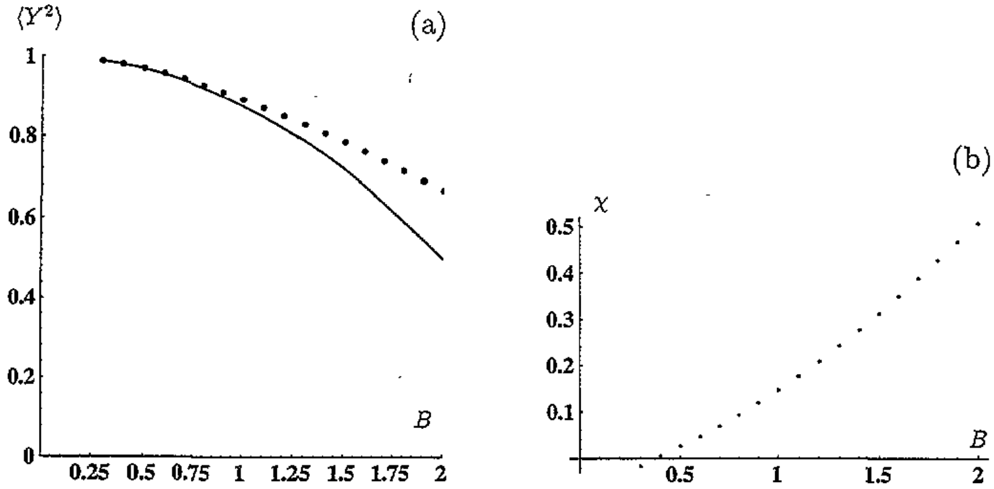

Figure 4. In (*a*), effective diffusivity $\langle Y^2\rangle$ as a function of barrier B. Period $A + B = 4$, shift $C = 0$, barrier B increasing from 0.30 to 2. Full circles: numerical results. Full curve: asymptotic formula $1 - B^2/(2A)$. In (*b*), relative error of the approximation using the asymptotic formula $\chi = (B^2/(2A) - (1 - \langle Y^2\rangle))/(1 - \langle Y^2\rangle)$.

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Appendix A

The numerical calculations require an integrated form of (3.1) because we divide straight lines into short intervals for the purpose of numerical integration. The probability that Brownian motion starting from $(x', 0)$ will hit the line segment $\{x = 0, y' < y < y''\}$ before hitting any other part of the y-axis is equal to

$$\int_{y'}^{y''} \frac{x'}{\pi((x')^2 + y^2)} \mathrm{d}y = \frac{1}{\pi}(\arctan(y''/x') - \arctan(y'/x')) . \tag{A.1}$$

We will discuss the transition probabilities corresponding to two cases in our sampling scheme. The first case is when the particle starts from a gate. In this case (see figure 2(*a*)) we have to calculate the probability $p(x'; v', v'')$ that a particle starting from a point $(x', 0)$ will hit a line segment $\{y = \pi/2, v' < x < v''\}$ before hitting any other part of the lines $\{y = \pm\pi/2\}$. The transformation (3.3) maps $(x', 0)$ onto $(\exp(x'), 0)$ and the line segment $\{y = \pi/2, v' < x < v''\}$ onto $\{x = 0, \exp(v') < y < \exp(v'')\}$. In view of (A.1),

$$p(x'; v', v'') = \frac{1}{\pi}(\arctan(\exp(v'')/\exp(x')) - \arctan(\exp(v')/\exp(x'))) . \tag{A.2}$$

By symmetry, the formula also applies to the case of hitting of the line segment $\{y = -\pi/2, v' < x < v''\}$.

Next we are going to discuss the case of the particle starting from above a barrier. This is equivalent (see figure 2(*b*)) to calculating the hitting probabilities for Brownian motion starting from a point $(x', 0)$ in the stripe $\{-\pi/2 < y < \pi/2\}$ without half-lines $\{y = 0, x < 0\}$ and $\{y = 0, x > B\}$. Let $p_1(x'; v', v'')$ be the probability that a particle starting from $(x', 0)$ will hit a line segment $\{y = \pi/2, v' < x < v''\}$ before hitting any other part of the boundary. We obtain a formula which is analogous to (A.2) except that we use (3.4) rather than (3.3) in its derivation:

$$p_1(x'; v', v'') = \frac{1}{\pi}\left[\arctan\left(\sqrt{\frac{(\exp(2v'') - 1)}{(\exp(2B) - \exp(2v''))}\frac{(\exp(2B) - \exp(2x'))}{(\exp(2x') - 1)}}\right) - \arctan\left(\sqrt{\frac{(\exp(2v') - 1)}{(\exp(2B) - \exp(2v'))}\frac{(\exp(2B) - \exp(2x'))}{(\exp(2x') - 1)}}\right)\right]. \tag{A.3}$$

Again, the symmetry implies that (A.3) also applies to hitting of the interval $\{y = -\pi/2, v' < x < v''\}$.

The situation is a bit more complicated when we consider the hitting of the interval $\{y = 0, v' < x < v''\}$ where either $v'' < 0$ or $v' > B$. If this interval lies on a barrier then (A.3) remains valid with the understanding that it represents the probability of hitting of the interval from one side, e.g. from above. However, if this interval lies in a gate, we have to double the probability given in (A.3) to account for the possibility that the particle may hit the interval from below or from above. We have to do so as we distinguish upper and lower sides of barriers but not gates.

Appendix B

We will show how (4.6) may be obtained from (4.3). Recall that $\tilde{x}$ is chosen so that $\hat{x} - \tilde{x}$ belongs to $\{y = 0, 0 < x < A + B\}$. Note that $\mathrm{d}x_k$, $x_1 - x_0$, $x_k - x_{k-1}$, and $P_2(x_{j-1}, x_j)$ for all j, will have the same values if we substitute $\hat{x}_j - \tilde{x}_0$ for $\hat{x}_j$ for all $j = 0, 1, 2$, etc. This follows from double periodicity of the system of barriers. Hence, (4.3) may be written as

$$\sum_{\beta_0}\sum_{n_1,\beta_1}\cdots\sum_{n_k,\beta_k}\int_{A_{\beta_0}}\mathrm{d}x_0\alpha(\hat{x}_0)\int\mathrm{d}x_1(x_1 - x_0)P_2(\hat{x}_0, \hat{x}_1)\int\mathrm{d}x_2P_2(\hat{x}_1, \hat{x}_2)\cdots \times\int\mathrm{d}x_k(x_k - x_{k-1})P_2(\hat{x}_{k-1}, \hat{x}_k). \tag{B.1}$$

Now we substitute $\hat{x}_j - \tilde{x}_1$ for $\hat{x}_j$ for all $j = 2, 3$, etc. Similar invariance properties imply that (B.1) is equal to

$$\sum_{\beta_0}\sum_{n_1,\beta_1}\sum_{n_2,\beta_2}\sum_{n_3,\beta_3}\cdots\sum_{n_{k-1},\beta_{k-1}}\sum_{n_k,\beta_k}\int_{A_{\beta_0}}\mathrm{d}x_0\alpha(\hat{x}_0)\int\mathrm{d}x_1(x_1 - x_0)P_2(\hat{x}_0, \hat{x}_1) \times\int\mathrm{d}x_2P_2(\hat{x}_1-\tilde{x}_1, \hat{x}_2-\tilde{x}_1)\int\mathrm{d}x_3P_2(\hat{x}_2, \hat{x}_3)\cdots\int\mathrm{d}x_k(x_k-x_{k-1})P_2(\hat{x}_{k-1}, \hat{x}_k). \tag{B.2}$$

The next substitution is $\hat{x}_j - (\hat{x}_2 - \tilde{x}_1)\check{}$ for $j = 3, 4$, etc. and also $\hat{x}_2 - \tilde{x}_1 - (\hat{x}_2 - \tilde{x}_1)\check{}$ for $\hat{x}_2 - \tilde{x}_1$. We obtain using the definition of Q

$$\sum_{\beta_0}\sum_{n_1,\beta_1}\sum_{\beta_2}\sum_{n_3,\beta_3}\cdots\sum_{n_{k-1},\beta_{k-1}}\sum_{n_k,\beta_k}\int_{A_{\beta_0}} \mathrm{d}x_0\alpha(\hat{x}_0)\int \mathrm{d}x_1(x_1-x_0)P_2(\hat{x}_0,\hat{x}_1)$$
$$\times\int_{A_{\beta_2}} \mathrm{d}x_2 Q(\hat{x}_1-\tilde{x}_1,\hat{x}_2)\int \mathrm{d}x_3 P_2(\hat{x}_2,\hat{x}_3)\cdots\int \mathrm{d}x_k(x_k-x_{k-1})P_2(\hat{x}_{k-1},\hat{x}_k)\,. \tag{B.3}$$

In order to obtain (4.6), we perform for $l = 3, 4, \ldots, k-1$ substitutions of $\hat{x}_j - \tilde{x}_l$ for $\hat{x}_j$ for all $j = l, l+1$, etc.

Appendix C

We will calculate the probability that a particle starting with the uniform distribution above a reflecting barrier of length ϵ on the line $\{y = 0\}$ will hit the line $\{y = \pi/2\}$ before hitting any part of the line $\{y = 0\}$ outside the barrier. Recall from section 3 that this is equivalent to calculating the probability that a particle starting with uniform distribution in a *gate* of length ϵ on the line $\{y = 0\}$ will hit one of the lines $\{y = \pm\pi/2\}$ before hitting any part of the line $\{y = 0\}$ outside the gate. We will use the transformation (3.4) which maps the stripe $\{-\pi/2 < y < \pi/2\}$ without two half-lines $\{y = 0, x < 0\}$ and $\{y = 0, x > \epsilon\}$ onto the half-plane $\{x > 0\}$. The hitting probabilities are invariant under this transformation. Under this transformation, the point $(p\epsilon, 0)$ is mapped onto

$$\sqrt{\frac{\exp(2p\epsilon)-1}{\exp(2\epsilon)-\exp(2p\epsilon)}}\,. \tag{C.1}$$

It is elementary to check that this expression converges to $\sqrt{p/(1-p)}$ when ϵ goes to zero. The mapping (3.4) transforms the uniform distribution in the gate into a distribution on the positive part of the real line. Let J have this last distribution. The probability that the starting point in the gate lies to the left of $p\epsilon$ is equal to p so the probability that J lies to the left of $\sqrt{p/(1-p)}$ is also equal to p, i.e.

$$P\big(J < \sqrt{p/(1-p)}\big) = p\,. \tag{C.2}$$

Let $x = \sqrt{p/(1-p)}$. Then $p = x^2/(1+x^2)$ and (C.2) may be expressed as

$$P(J < x) = x^2/(1+x^2)\,. \tag{C.3}$$

The density of J is equal to

$$\frac{\mathrm{d}}{\mathrm{d}x}P(J < x) = \frac{2x}{(1+x^2)^2}\,. \tag{C.4}$$

The transformation (3.4) maps the lines $\{y = \pm\pi/2\}$ onto line segments $\{x = 0, \mathrm{e}^{-\epsilon} < y < 1\}$ and $\{x = 0, -1 < y < -\mathrm{e}^{-\epsilon}\}$. According to (B.1), the probability of hitting one of these segments before hitting any other part of the y-axis while starting from $(x, 0)$ is equal to

$$(2/\pi)(\arctan(1/x) - \arctan(e^{-\epsilon}/x)) . \tag{C.5}$$

Since $e^{-\epsilon} = 1 - \epsilon + o(\epsilon)$ the last expression is approximately equal to

$$(2/\pi)(\arctan(1/x) - \arctan((1-\epsilon)/x)) . \tag{C.6}$$

We have

$$\frac{d}{dy} \arctan(y/x)|_{y=1} = x/(x^2 + y^2)|_{y=1} = x/(1 + x^2) . \tag{C.7}$$

Hence, (C.6) is approximately equal to

$$\frac{2\epsilon x}{\pi(1+x^2)} . \tag{C.8}$$

The desired probability is obtained by integrating this probability over the positive real axis with the density function (C.4). We obtain

$$\begin{aligned} \int_0^\infty \frac{2\epsilon x}{\pi(1+x^2)} \frac{2x}{(1+x^2)^2} dx &= \frac{4\epsilon}{\pi} \int_0^\infty \frac{x^2}{(1+x^2)^3} dx \\ &= \frac{4\epsilon}{\pi} \left(\frac{x}{8(1+x^2)} - \frac{x}{4(1+x^2)^2} + \arctan(x)/8 \right) \Bigg|_{x=0}^{x=\infty} = \epsilon/4 . \end{aligned} \tag{C.9}$$

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