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2D Brownian motion in a system of traps: application of conformal transformations

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Abstract. We study two-dimensional Brownian motion in a periodic system of traps using conformal transformations. The system is periodic in the x and y directions. We calculate the ratio of the drift along the y-axis to the drift along the x-axis. The drift of the Brownian particle is induced by conditioning and by the asymmetry of the system of traps. Finally we find the placement of traps which gives the maximal drift ratio.

1. Introduction

Brownian motion in the presence of 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]. Here we would like to consider a two-dimensional (2D) Brownian motion in a periodic system of linear absorbing traps, as shown in figure 1(a). The period of the system of traps is nQ in the x direction and $n\pi$ in the y direction. The distance between the lines of traps is π and the size of a gate between the traps on a single line is P. Here P, Q and n are parameters, satisfying $nQ > P$; we consider only integer n in order to simplify computations. Whenever the Brownian trajectory hits a black line (trap) it is absorbed, so it can only move through the gates. The Brownian particle, conditioned to hit the line $x = -\infty$ without being absorbed, will have a steady drift induced by the conditioning and the absorbing traps. The easy way to visualize how the absorbing traps induce drift is to consider the one-dimensional (1D) case with one absorbing barrier on a line. In this 1D case, the single absorbing barrier effectively repels the centre of the probability distribution for a conditioned Brownian particle. In our 2D system, the centre of the probability distribution for a conditioned Brownian particle will move in the direction of the solid line, indicated in figure 1(a) for a particular case of $n = 3$.

The problem we pose here is: for a given integer value of n, what are the values of P and Q which maximize the ratio of the drift along y-axis to the one along the x-axis? This ratio, which we denote λ, is equal to $\tan\theta$, where the angle θ is shown in figure 1(a). Note that in the particular case of $n = 1, 2$ the drift along y-axis is zero

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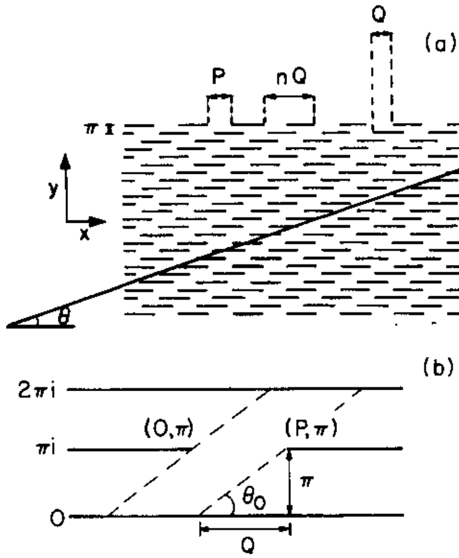

Figure 1. (a) The periodic system of traps with period nQ along the x-axis and period $n\pi$ along y-axis for a particular case with $n=3$. The size of the gate is P whereas the distance between two neighbouring lines of gates is π. The solid line denotes the direction of the drift of the conditioned Brownian particle. (b) The basic unit of the structure shown in (a). A double stripe with a single gate in the middle. The dashed lines indicate the channel formed by the gates shown in (a). θ_0 is the inclination of the channel formed by the gates ($\tan\theta_0=\pi/Q$).

due to the symmetry of the trap system. Thus the first non-trivial case is obtained for $n=3$. In order to study the problem we will employ the conformal invariance of Brownian motion [9], i.e. the invariance of Brownian motion under local rotations and local changes of spatial and temporal scale. The conformal invariance property has been a working tool in the case of 2D critical systems [10] and in 2D polymer systems modelled as self-avoiding random walks [11]. Here we will use this property to obtain various probability densities for our system, by applying analytic mappings (conformal transformations) of the complex plane onto itself. In this way we can transform a complicated system of traps onto a much simpler one, where all the interesting probability densities are easy to obtain, and then transform it back to our original system.

The paper is arranged as follows. In section 2 we will use conformal transformations to obtain the density of the hitting (probability) distribution (or density of harmonic measure [12]) for the stripe shown in figure 1(b). In section 3, we use this density to compute those of the hitting distribution and the stationary probability distribution for the conditioned process. The results and the discussion are presented in section 4.

2. Density of hitting distribution

From now on it will be convenient to use the complex variables $z=x+iy$. From figure 1(a) we see that the basic building block of our system of traps is a double stripe with a single gate in the middle, as shown in figure 1(b). Consider where the Brownian trajectory, starting from any point in this gate, will for the first time hit any of the black lines forming the boundary of the stripe. Let $h(z, z')\,dz'$ denote the probability that it hits in the interval $z' \pm dz'/2$, starting from z. Here $z = x + \pi i$ for some $x \in (0, P)$, and z' has the form $w + 2\pi i$ or w or $w + \pi i$, where w is real. The function h so defined is called the density of the hitting distribution, or DHD. A way of computing this density is shown in figure 2. The simple family of conformal transformations (analytic mappings) shown there maps the stripe onto a circle [13]. The density of the hitting distribution must transform accordingly since Brownian motion is conformally invariant [14]. For the circle, we know by symmetry that $h(z, z') = 1/(2\pi|z - z'|)$, where $|z - z'| = r$ is the radius of the circle, z corresponds to the centre of the circle and z'

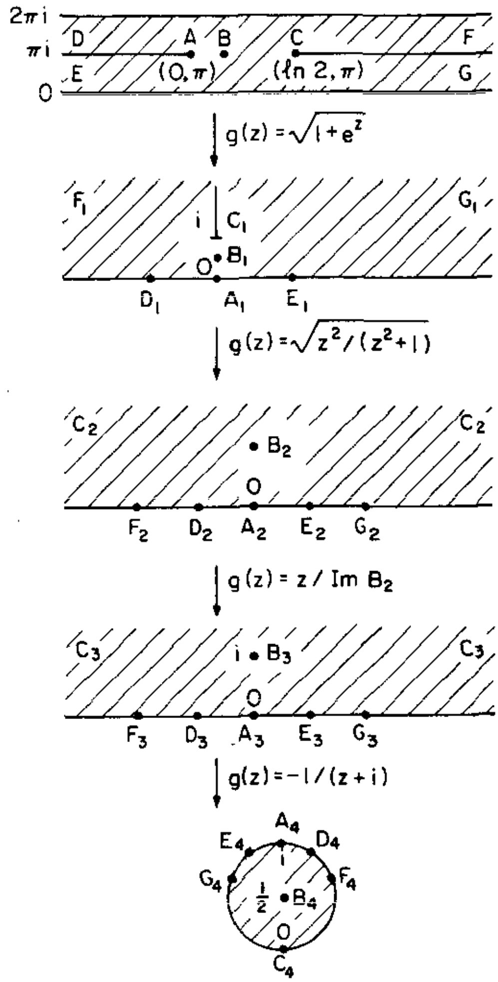

Figure 2. A family of conformal transformations mapping the double stripe with a single gate in the middle onto a circle. Only the case $P = \log 2$ is illustrated. Other cases may be treated in a similar way. We choose the branch of the square root for which we have $\sqrt{z} = \exp((1/2)\log z)$ and $\operatorname{Im}\log z \in (0, 2\pi)$. The point A is mapped successively onto A_1, A_2, A_3, A_4 and the same remark applies to B, C, etc. We have $B = x + \pi i$, $B_1 = \sqrt{1 - e^x}$, $B_2 = \sqrt{(1 - e^x)(2 - e^x)}$, $\operatorname{Im} B_2 = \sqrt{(e^x - 1)(2 - e^x)}$, $E_1 = 1$, $E_2 = 1/\sqrt{2}$, $E_3 = 1/\sqrt{2(e^x - 1)(2 - e^x)}$, $E_4 = -1/(i + 1/\sqrt{2(e^x - 1)(2 - e^x)})$, $G_2 = 1$, $G_3 = 1/\sqrt{(e^x - 1)(2 - e^x)}$, $G_4 = -1/(i + 1/\sqrt{(e^x - 1)(2 - e^x)})$. Other values may be obtained by symmetry.

lies on its circumference. In general, if the DHD for system 0 is $f_0(z, z')$, and the transformation $w = g(z)$ maps system 1 onto system 0, then the DHD for system 1 is

$$f_1(z, z') = f_0(g(z), g(z'))\left|\frac{\mathrm{d}g(z')}{\mathrm{d}z'}\right|. \tag{2.1}$$

Using the transformations shown in figure 2 and some elementary scaling we arrive at the following formula for $h(z, z')$, for the stripe shown in figure 1(b) (here $x \in (0, P)$):

$$h(x+\pi\mathrm{i}, w+2\pi\mathrm{i}) = h(x+\pi\mathrm{i}, w) = f_4(x, w) \tag{2.2}$$

$$h(x+\pi\mathrm{i}, w+\pi\mathrm{i}) = \begin{cases} 2\tilde{f}_4(x, w) & \text{if } w<0 \\ 2\tilde{f}_4(P-x, P-w) & \text{if } w>P \end{cases} \tag{2.3}$$

where

$$f_4(x, w) = \frac{\exp w\sqrt{-1+\exp x}\,\sqrt{1-\exp x+c^2}}{2\pi(\exp x+\exp w)\sqrt{1+\exp w}\,\sqrt{1+\exp w+c^2}} \tag{2.4}$$

$$\tilde{f}_4(x, w) = \frac{\exp w\sqrt{-1+\exp x}\,\sqrt{1-\exp x+c^2}}{2\pi(\exp x-\exp w)\sqrt{1-\exp w}\,\sqrt{1-\exp w+c^2}} \tag{2.5}$$

and

$$c = \sqrt{\exp P - 1}. \tag{2.6}$$

The factor of 2 in (2.3) comes from the fact that the trajectory can reach the middle line in the stripe shown in figure 1(b) from two sides.

A more physical interpretation of DHD, $h(x+2\pi\mathrm{i}, w+2\pi\mathrm{i})$, is that as the solution of the diffusion equation for a density with a single source inside the gate at $x+2\pi\mathrm{i}$, and with the boundary condition of zero density at the black lines (this is analogous to the problem discussed in [3]). Our function $h(x+2\pi\mathrm{i}, w+2\pi\mathrm{i})$ is proportional to the norm of the current at the boundary at $w+2\pi\mathrm{i}$, which is equal to the gradient of the density field [15] at this point.

In the next section we will use the DHD to calculate the density of the conditional hitting distribution (DCHD). The process is conditioned in such a way that all its trajectories reach the line $x=-\infty$ without hitting a trap.

3. Density of conditional hitting distribution

The renormalized probability that the Brownian trajectory starting at z will eventually reach the line $x=-\infty$ without hitting the trap is denoted $\mu(z)$. This function satisfies the following equation involving the DHD (see figure 1):

$$\begin{aligned}\mu(x+\pi\mathrm{i}) = &\sum_{k=-\infty}^{\infty}\int_0^P \mathrm{d}w\, h(x+\pi\mathrm{i}, w-Q+nkQ)\mu(w-Q+nkQ)\\ &+\sum_{k=-\infty}^{\infty}\int_0^P \mathrm{d}w\, h(x+\pi\mathrm{i}, w+Q+nkQ+2\pi\mathrm{i})\mu(w+Q+nkQ+2\pi\mathrm{i})\\ &+\sum_{\substack{k=-\infty\\ k\neq 0}}^{\infty}\int_0^P \mathrm{d}w\, h(x+\pi\mathrm{i}, w+nkQ+\pi\mathrm{i})\mu(w+nkQ+\pi\mathrm{i}).\end{aligned} \tag{3.1}$$

This equation can be interpreted as follows: the trajectory, which starts at a gate at point $z=x+\pi\mathrm{i}$, will reach infinity without hitting a trap, only if it first reaches one of the gates located on the neighbouring lines or on the same line. The chance of reaching the line $x=-\infty$ without hitting another gate is negligible. The probability of reaching a point z' in a new gate is given by $h(z, z')$. Once in the new gate the trajectory has a new probability $\mu(z')$ of reaching infinity, which depends on the location of the hitting point z' in the new gate. The traps and the starting gate (corresponding to $k=0$ in the third term of the left-hand side of (3.1)) are of course excluded from the sums. Let $x, y \in (0, P)$. The ratio of $\mu(z)$ at $z=x+nkQ+\pi\mathrm{i}$ to $\mu(z')$ at $z'=y-Q+nk'Q$ or $z'=y+Q+nk'Q+2\pi\mathrm{i}$ or $z'=y+nk'Q+\pi\mathrm{i}$ is given as follows:

$$\frac{\mu(z)}{\mu(z')}=\frac{\gamma(x)}{\gamma(y)}\exp(A(\mathrm{Re}(z-z'))). \tag{3.2}$$

Equation (3.2) constitutes a definition of the function $\gamma(x)$ and the constant A. Because $\gamma(x)$ is defined up to a multiplicative constant, we additionally impose a normalization condition of $\gamma(x)$, i.e.

$$\int_0^P \mathrm{d}x\, \gamma(x)=1. \tag{3.3}$$

Both the constant A and the normalized function $\gamma(x)$ have to be determined from (3.1). If A satisfies (3.1) together with some $\gamma(x)$ so does $-A$. We choose the negative A because the system is conditioned to reach line $x=-\infty$. The positive solution corresponds to the trajectories which reach $x=\infty$. This symmetry is due to the inverse symmetry of h. Equation (3.2) can be justified rigorously; here we only note that this equation implies the exponential spatial rate of absorption. Finally the density of the conditional hitting distribution is

$$h_\mu(z, z')=\frac{\mu(z')}{\mu(z)}h(z, z'). \tag{3.4}$$

Equation (3.4) follows from the definition of conditional probability [16]. This new density, $h_\mu(z, z')$, corresponds to the class of all trajectories (conditioned Brownian process [17]) which reach infinity without hitting a trap. The conditioned Brownian process has a stationary probability distribution for hitting points in any single gate. Its density $\alpha(z)$ satisfies the following equation:

$$\begin{aligned}\alpha(w+\pi\mathrm{i})=\int_0^P \mathrm{d}x\bigg(&\sum_{k=-\infty}^{\infty} h_\mu(x+\pi\mathrm{i}, w-Q+nkQ)\\ &+\sum_{k=-\infty}^{\infty} h_\mu(x+\pi\mathrm{i}, w+Q+nkQ+2\pi\mathrm{i})\\ &+\sum_{\substack{k=-\infty\\ k\neq 0}}^{\infty} h_\mu(x+\pi\mathrm{i}, w+nkQ+\pi\mathrm{i})\bigg)\alpha(x+\pi\mathrm{i})\end{aligned} \tag{3.5}$$

together with the normalization condition for $\alpha(z)$, i.e.

$$\int_0^P \mathrm{d}x\, \alpha(x+\pi\mathrm{i})=1. \tag{3.6}$$

This quantity tells us how the hitting points of the trajectories of the conditioned Brownian process are distributed in a gate. Then the drift $\lambda = \tan\theta$ (figure 1(*a*)) is defined as:

$$\lambda = V/H \tag{3.7}$$

where V is the drift along y and H is the drift along x. They are defined as averages over the trajectories of the conditioned Brownian process between consecutive hits of the gates, namely,

$$V = -\pi \sum_{k=-\infty}^{\infty} \int_0^P \int_0^P \mathrm{d}x\, \mathrm{d}w\, h_\mu(x+\pi\mathrm{i}, w-Q+nkQ)\alpha(x+\pi\mathrm{i}) + \pi \sum_{k=-\infty}^{\infty} \int_0^P \int_0^P \mathrm{d}x\, \mathrm{d}w\, h_\mu(x+\pi\mathrm{i}, w+Q+nkQ+2\pi\mathrm{i})\alpha(x+\pi\mathrm{i}) \tag{3.8}$$

and

$$\begin{aligned} H = {} & \sum_{k=-\infty}^{\infty} \int_0^P \int_0^P \mathrm{d}x\, \mathrm{d}w\, h_\mu(x+\pi\mathrm{i}, w-Q+nkQ)\alpha(x+\pi\mathrm{i})(w-Q+nkQ-x) \\ & + \sum_{k=-\infty}^{\infty} \int_0^P \int_0^P \mathrm{d}x\, \mathrm{d}w\, h_\mu(x+\pi\mathrm{i}, w+Q+nkQ+2\pi\mathrm{i}) \\ & \times \alpha(x+\pi\mathrm{i})(w+Q+nkQ-x) \\ & + \sum_{\substack{k=-\infty \\ k\neq 0}}^{\infty} \int_0^P \int_0^P \mathrm{d}x\, \mathrm{d}w\, h_\mu(x+\pi\mathrm{i}, w+nkQ+\pi\mathrm{i}) \\ & \times \alpha(x+\pi\mathrm{i})(w+nkQ-x). \end{aligned} \tag{3.9}$$

Of course the summation as in the case of (3.1) runs over all the gates except for one ($k \neq 0$). In the next section we present the results of numerically solving (3.1)-(3.9).

4. Results and discussion

We performed calculations from $n=3$ to $n=50$ in increments of 1 and from $n=50$ to $n=200$ in increments of 10. For larger values of n the numerical difficulties vitiated the calculations. For each n we found the values of P and Q for which the ratio λ was maximal. The results are summarized in figure 3 (figures 3-5 refer to the case of the *maximal drift ratio*). In figure 3(*a*) the maximal value of $\lambda = \tan\theta$, minus $\tan\theta_0 = \pi/Q$, is plotted against n. For large n we find the following asymptotic relation for θ and Q corresponding to the maximal drift ratio:

$$\tan\theta = \frac{\pi}{Q} - \delta \tag{4.1}$$

$$\delta = 0.075 \pm 0.008. \tag{4.2}$$

Note that $\tan\theta$ (figure 1(*a*)) is almost equal to $\tan\theta_0$ (the angle θ_0 is shown in figure 1(*b*)). Equations (4.1) and (4.2) and figure 3(*a*) show the correction to this equality. For large n, Q is rather small and when n goes to infinity, Q goes to zero (figure 3(*b*)). Thus in this limit ($n=\infty$) δ constitutes a negligible correction. This correction cannot

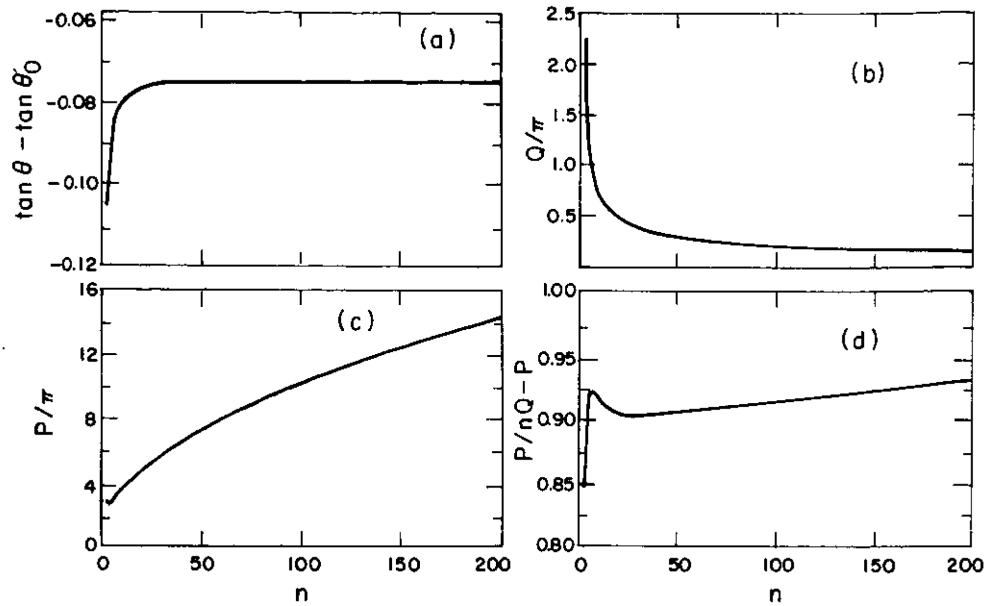

Figure 3. (a) The maximal drift ratio, $\tan\theta$ (angle θ shown for $n=3$ in figure 1(a)) minus $\tan\theta_0$ (angle θ_0 shown in figure 1(b)) versus n. Their difference reaches asymptotic value of $\delta = 0.075 \pm 0.008$ for very large n. For eye guidance the discrete points (n is integer) have been joined by a continuous line. (b) The ratio of Q to the distance between the lines of traps, π, versus n for the maximal drift ratio. (c) The ratio of the size of the gate, P, to the distance between the lines of traps, π, versus n for the maximal drift ratio. (d) The ratio of the size of the gate, P, to the size of the trap, $nQ-P$, versus n for the maximal drift ratio.

be neglected for small n as can be seen from figure 1(a), where the system of traps and the line of drift have been presented for the case of $n=3$. Without the correction the drift would follow a channel of gates without crossing the traps. In figure 3(c) P versus n is shown for the distribution of traps which give the maximal drift ratio. Finally figure 3(d) shows the ratio of the size of the gate, P, to the size of the trap, $nQ-P$ for the maximal drift ratio. For all n studied, we find the maximal drift ratio when the size of a trap is about ten per cent larger than the size of a gate. This gate size–trap size ratio is a non-monotonic function of n. First, it grows for $3<n<7$, attaining a local maximum at $n=7$. Then it decreases down to the local minimum at $n \approx 30$ and finally it grows very slowly for $33<n<200$. Numerical uncertainty does not allow us to draw conclusions regarding the exact dependence of this growth on n. Figure 4 and figure 5 show the constant A (equation (3.2)) and the density function α for a single gate, respectively. The constant A is negative and is a non-monotonic function of n. It has a local maximum at $n \approx 30$, at the same place as the minimum of gate size–trap size ratio $P/(nQ-P)$ (figure 3(d)). Then it decreases very slowly with n. The density function $\alpha(x)$ is very asymmetric with respect to the centre of the gate for small n, but evolves quickly towards a symmetric distribution. It is essentially symmetric by $n = 100$.

In summary we have studied two-dimensional conditioned Brownian motion in a periodic system of traps. We have determined the distribution of traps which maximizes the ratio of the drift along y to the drift along x. In order to do so we had to calculate

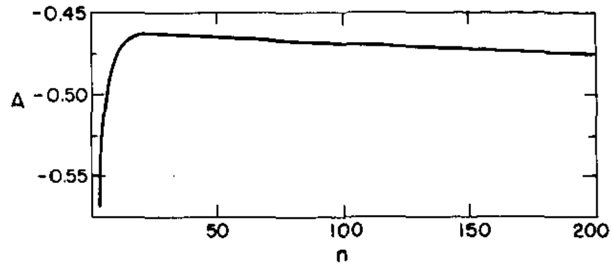

Figure 4. The parameter A versus n for the maximal drift ratio.

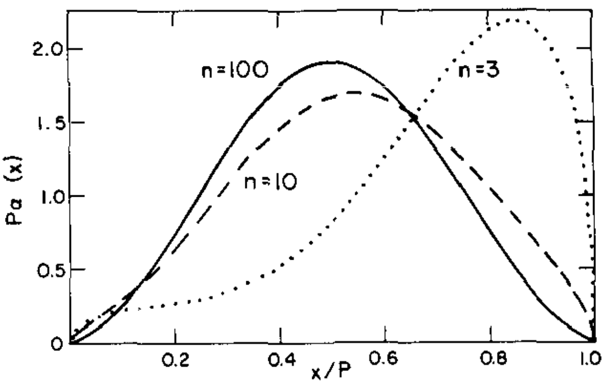

Figure 5. *The evolution, with n, of the stationary distribution for the conditioned Brownian* process in a single gate for the maximal drift ratio (figures 3, 4). Here x measures distance within the gate and P, for a given n, is equal to its value shown in figure 3(c). Dotted line, $n=3$, dashed line, $n=10$ and solid line, $n=100$.

the densities of various probability distributions, using conformal transformations. We hope that both our results and the presented method will be helpful for future studies of 2D Brownian motion in various systems of traps. In particular we hope that our results will find applications in the physical problems mentioned in the introduction. Diffusion limited aggregation, percolation, and diffusion in porous media are all situations in which particles are moving in some region with microscopic (local) barriers either absorbing or reflecting or the combination of both [15]. In models where the distribution of traps is completely random as we believe would be the case for porous media, it is hard to calculate the stochastic properties of the system. We give here a simpler model where the system of traps is distributed periodically in space and where certain theoretical predictions can be made. We hope to extend our analysis to more complicated distributions of traps including random distributions. Then we hope to make some definitive predictions for the physical systems such as diffusion limited aggregation or diffusion in porous media.

Acknowledgments

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