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Some Properties of the Asymptotic Solutions of the Montroll–Weiss Equation

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Curves of asymptotic probability densities appropriate to the continuous-time random walk model of Montroll and Weiss are presented and are calculated numerically using the fast Fourier transform. The behavior of the moments is briefly discussed and it is shown that the Einstein formula relating the diffusion and mobility coefficients can be generalized to include the case where the mean waiting time between hops is infinite.

KEY WORDS: Random walk; diffusion; mobility; stable distribution.

1. INTRODUCTION

In a previous paper Tunaley(1) derived the asymptotic probability densities for random walks based on the continuous-time model of Montroll and Weiss.(2) A scaling process is employed so that as time progresses the scale of length is expanded. In the limit, the shape of the distribution or density curve is unchanged by the scaling (given certain conditions of regular variation in the underlying densities) and it is shown that the limiting forms can be expressed in terms of the stable densities. Both symmetric walks, appropriate to pure diffusion, and asymmetric walks, relevant to diffusion with drift, are covered. In all cases the mean and variance of the distance traveled in one hop are finite while the waiting time between hops may have infinite

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Table I

Exponent		
Symmetric diffusion $0 < \nu < 1$	$P\left\{\frac{X}{\sigma_0} > x, t\right\} = \frac{1}{2} S_{\nu/2}\left[\frac{t}{(2\alpha x^2)^{1/\nu}}\right],$	$x > 0$
	$P\left\{\frac{X}{\sigma_0} < x, t\right\} = \frac{1}{2} S_{\nu/2}\left[\frac{t}{(2\alpha x^2)^{1/\nu}}\right],$	$x < 0$
$1 < \nu \leqslant 2$	(Normal with variance $2Dt = \sigma^2 t/\alpha$)	
	$P\left\{\frac{X}{\sigma_0} > x, t\right\} = \frac{1}{2} S_{1/2}\left[\frac{t}{2\sigma x^2}\right],$	$x > 0$
	$P\left\{\frac{X}{\sigma_0} < x, t\right\} = \frac{1}{2} S_{1/2}\left[\frac{t}{2\alpha x^2}\right],$	$x < 0$
Asymmetric diffusion		
$0 < \nu < 1$	$P\left\{\frac{X}{\mu} > x, t\right\} = S_\nu\left[\frac{t}{(\alpha x)^{1/\nu}}\right],$	$x > 0$
	$P\left\{\frac{X}{\mu} < 0, t\right\} = 0,$	$x < 0$
$1 < \nu < 2$	$P\left(X > \frac{\mu t}{\alpha} - \frac{\mu x}{\alpha}\left(\frac{\beta t}{\alpha}\right)^{1/\nu}\right) = S_\nu(x)$	
$\nu = 2$	Normal distribution with mean distance $\mu t/\alpha$ and variance $2D't = (\sigma^2 - 2\mu^2 + \mu^2\beta/\alpha^2)t/\alpha$	

mean or variance. The results are shown in Table I. Here the same notation is used as in Ref. 1: μ, σ_0^2, and σ^2 are the mean, variance, and mean square distances covered in one hop; α and β are scale constants in the distribution of the waiting time. S_ν represents a stable distribution with zero centering, unit scale parameter, and exponent ν. When $1 < \nu < 2$ it is two-sided but asymmetric.

A fast Fourier transform program was employed to compute the stable densities from their characteristic functions directly, using 1024 points for $1 < \nu \leqslant 2$ and 8192 points for $0 < \nu < 1$. The characteristic functions, with unit scale parameters, are

$$\begin{aligned} &\exp[-|\omega|^\nu \exp(\pm i\pi\nu/2)], \qquad 0 < \nu < 1 \\ &\exp[|\omega|^\nu \exp(\pm i\pi\nu/2)], \qquad 1 < \nu \leqslant 2 \end{aligned} \tag{1}$$

where the plus signs apply when $\omega \leqslant 0$ and the minus signs when $\omega > 0$. In the case $\nu = 2$ we have a normal density with variance equal to two.

The results for $0 < \nu < 1$ were checked for large times by employing the Tauberian theorem[3] on the Laplace transform equivalent to Eq. (1).

Figures 1–3 show the one-sided densities corresponding to $S_\gamma(x^{-1/\gamma})$ for $\gamma = 0.4$, 0.5, and 0.8, respectively. For pure diffusion with $0 < \nu < 1$ only the first curve is relevant and should be reflected about the origin (the factor $\frac{1}{2}$ necessary for normalization should be included). It should be noted that the result of this symmetrization is not equivalent to the use of a "symmetric stable distribution," which has characteristic function $\exp(-|\omega|^\nu)$. It is evident that the density for $\nu = 0.8$ ($\gamma = 0.4$) is somewhat more peaked at the origin than the normal curve, which is actually reproduced when the density corresponding to $\gamma = 0.5$ is symmetrized. This latter naturally applies when $\nu = 2$ and also when $1 < \nu < 2$ (see Table 1).

On the other hand, when drift is present there is a qualitative difference between the densities according to whether $\nu < \frac{1}{2}$ or $\frac{1}{2} < \nu < 1$. For the former case the density is the one-sided version of the diffusion curve and exhibits a sharp step at the origin to its peak value, while for the latter, again we have a step at the origin but the maximum occurs at a finite distance. The step is due to the significant probability that in time t some particles have not performed any jump. For example, the asymptotic result gives

$$p(0, t)\,dx = \alpha\,dx/\mu t^\nu \Gamma(1 - \nu) \tag{2}$$

(to arrive at this, the Tauberian theorem can be used to find the behavior of a stable density at large times[3]). However, from first principles, if the

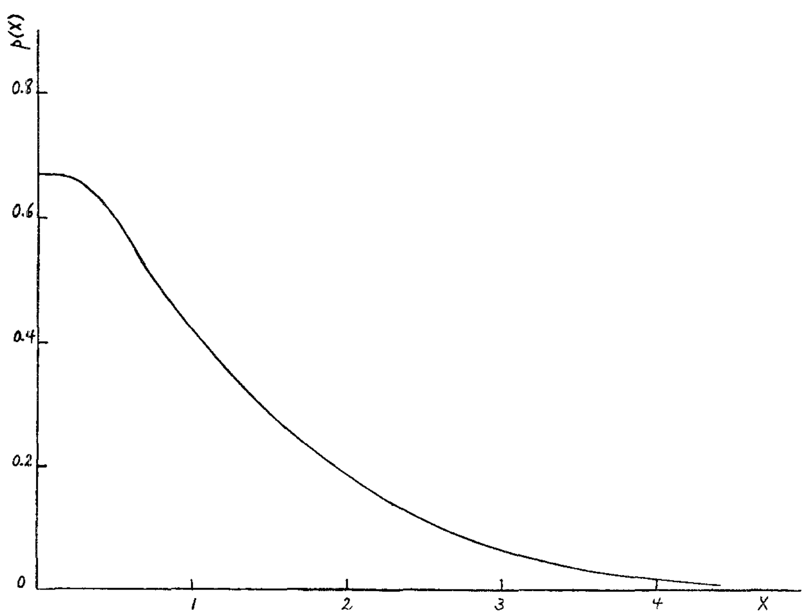

Fig. 1. The density corresponding to the stable distribution $S_{0.4}(x^{-2.5})$.

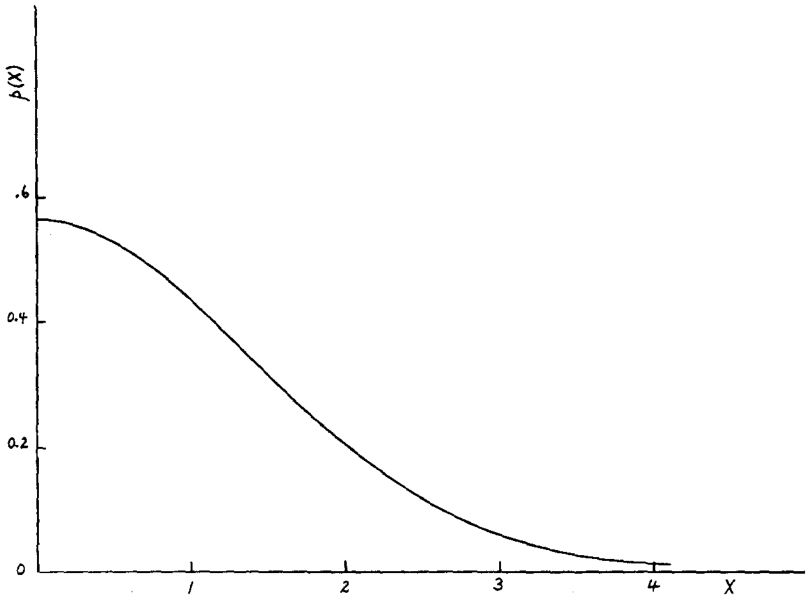

Fig. 2. The density corresponding to the stable distribution $S_{0.5}(x^{-2})$.

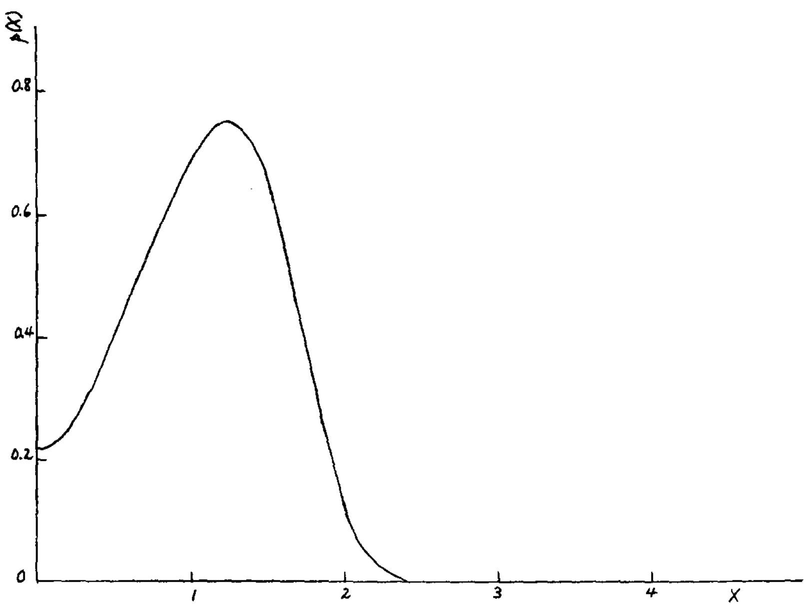

Fig. 3. The density corresponding to the stable distribution $S_{0.8}(x^{-1.25})$.

distribution of waiting times is $F(t)$, the probability that there has been no jump in time t is

$$P[T > t] = 1 - F(t) \tag{3}$$

But the original postulate in Ref. 1 was

$$1 - F(t) = \alpha/t^{\nu}\Gamma(1 - \nu), \qquad t \to \infty \tag{4}$$

so that, since a particle is located typically over a distance μ, we have essentially the same result as Eq. (2). This behavior is similar to that calculated by Montroll and Sher[4] for those of their waiting time densities, which have the asymptotic form

$$(\pi)^{-1/2}t^{-3/2} \tag{5}$$

which shows that $\nu = \frac{1}{2}$ is appropriate and the results correspond to Fig. 2.

For $1 < \nu < 2$ with drift, the density is that of an asymmetric stable density with a long tail toward the origin. This density drifts with a velocity μ/α. The curves shown in Figs. 4–6 for $\nu = 1.2$, 1.5, and 1.9 are asymmetric stable densities with their centering at the origin, unit scale factor, and the long tail on the positive half-axis (to represent drift from left to right, they should be turned around). One of the main points of interest is the fact that their peaks do not lie at the origin, unlike the normal density.

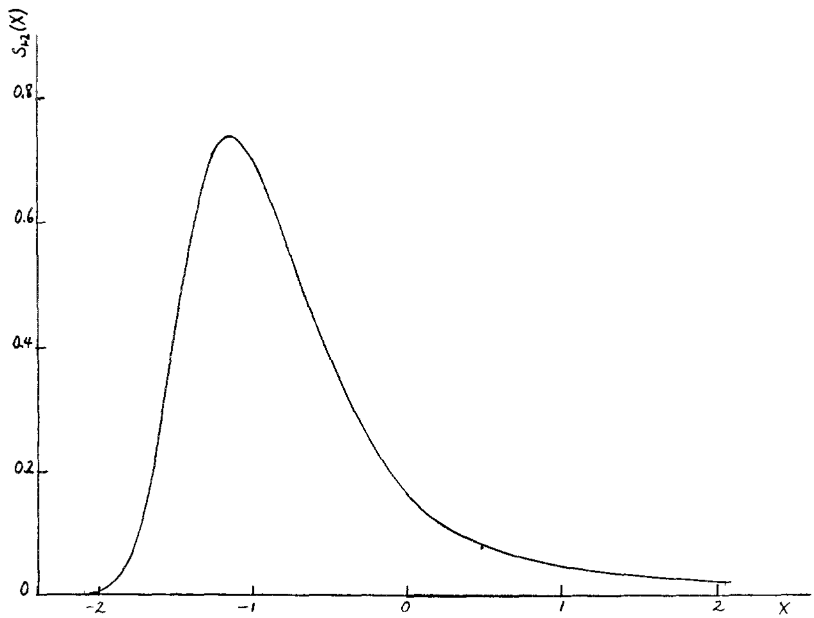

Fig. 4. The density corresponding to the asymmetric stable distribution $S_{1.2}(x)$.

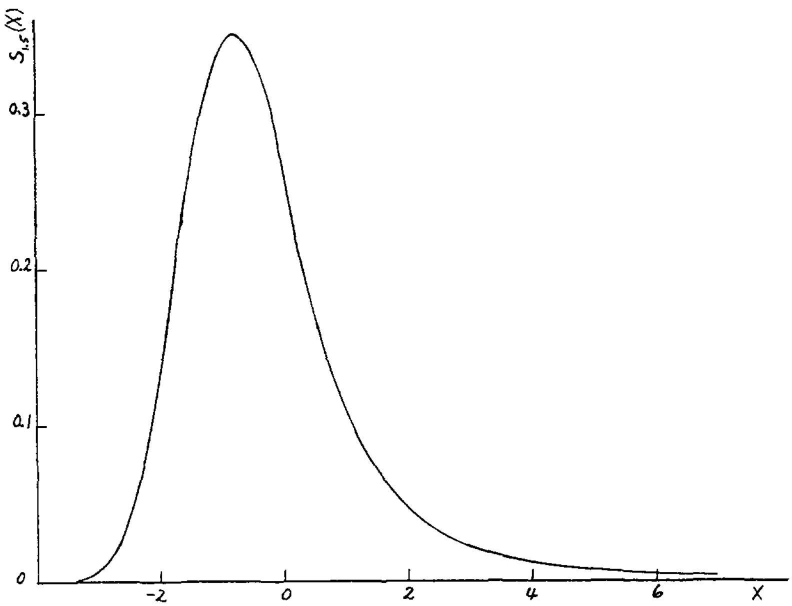

Fig. 5. The density corresponding to the asymmetric stable distribution $S_{1.5}(x)$.

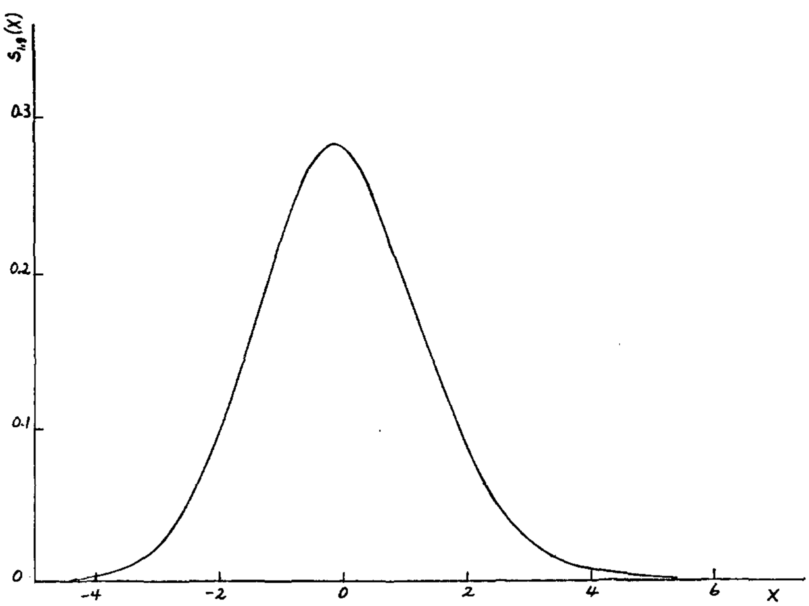

Fig. 6. The density corresponding to the asymmetric stable distribution $S_{1.9}(x)$.

2. GROSS BEHAVIOR

The mean and variance of the distance covered in time t for large t have been examined by Shlesinger.[5] His results are more general than those to be presented here but the same technique can be applied. For example, the Laplace transform of the mean distance can be found by differentiating the Montroll–Weiss (MW) equation:

$$\langle x(s)\rangle = -i[\partial p(k, s)/\partial k]_{k=0} \tag{6}$$

It is easily verified that we can let $t \to \infty$ in Shlesinger's equations and obtain the same result as by differentiating the asymptotic MW transforms: For $0 < \nu < 1$ we have for pure diffusion

$$\langle x(t)\rangle = 0 \tag{7}$$

$$\langle x^2(t)\rangle = \sigma^2 t^\nu/\alpha\Gamma(1 + \nu) \tag{8}$$

while for $0 < \nu < 1$ and asymmetric diffusion

$$\langle x(t)\rangle = \mu t^\nu/\alpha\Gamma(1 + \nu) \tag{9}$$

$$\langle x^2(t)\rangle = 2\mu^2 t^{2\nu}/\alpha^2\Gamma(1 + 2\nu) \tag{10}$$

As pointed out by Shlesinger, the behavior of asymmetric diffusion is unusual for $0 < \nu < 1$ in that the dispersion (standard deviation) grows as quickly as the mean.

For $1 < \nu < 2$ the situation is quite different. For symmetric diffusion the density is normal with variance given by $\sigma^2 t/\alpha$ (the diffusion coefficient is $\sigma^2/2\alpha$). With a drift the density has a velocity μ/α and if $\nu = 2$, the variance is

$$(\sigma^2 - 2\mu^2 + \mu^2\beta/\alpha^2)t/\alpha \tag{11}$$

However, if $1 < \nu < 2$, the variance is apparently infinite (we must bear in mind that this really means that as $t \to \infty$ the variance tends to infinity). Nevertheless, we can still employ the properties of stable distributions to note that the dispersion as measured by the half-width (say) varies as $t^{1/\nu}$, by an examination of Eq. (57) in Ref. 1. Thus the dispersion grows faster than that for ordinary diffusion ($t^{1/2}$).

3. EINSTEIN RELATION

The Einstein relation expresses the fact that for a system exhibiting a linear response the ordinary diffusion coefficient D is related to the mobility K, i.e.,

$$D = kTK \tag{12}$$

where k is Boltzmann's constant and T is the temperature. It is evident that for well-defined coefficients to exist we must move into the realm of asymptotic behavior. If a mean hopping time exists ($1 < \nu < 2$), the mobility can be expressed readily in terms of microscopic parameters. Defining

$$K = \langle \text{drift velocity} \rangle / F \tag{13}$$

where F is the applied force on the particle, yields

$$K = \mu / \alpha F$$

On the other hand, for diffusion in the absence of a field and again for $1 < \nu < 2$

$$D = \sigma_0^2 / 2\alpha$$

Thus

$$D/K = \sigma_0^2 F / 2\mu \tag{14}$$

To make full use of the MW formulation the following model is introduced. A one-dimensional string of potential barriers of equal heights is set up with the condition that the distances between the centers of neighboring wells are independent random variables. A particle naturally sits mainly in the center of a well, but, since we shall assume that it is essentially in thermodynamic equilibrium within any particular well, it is subject to the thermal agitation of the lattice and has a small probability of jumping over the barriers into the wells on either side. It will be deemed to be making a transfer if it is found at the top of a barrier (see Fig. 7). The distances between the tops of the barriers are denoted by x_j: Unfortunately, if the distances between well centers are independent, the x_j will usually not be.

From the theory of statistical thermodynamics we know that the probability of the particle's being found at the top of the barrier of the jth well is proportional to

$$\exp(\pm F x_j / 2kT) \tag{15}$$

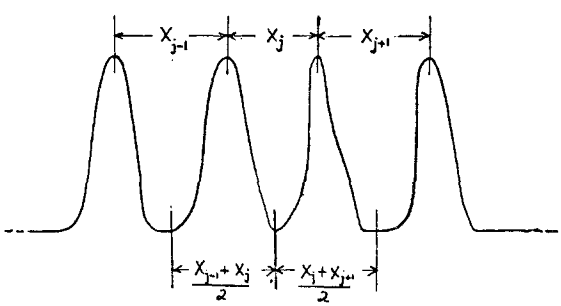

Fig. 7. The model of random potential barriers.

where the plus sign is appropriate to the barrier in the direction of the applied field and the minus sign to the reverse direction. By the earlier definition these probabilities are proportional to the probabilities of transfer. Only two outcomes are relevant, so that normalizing and expanding in small F (linear response) yields

$$\begin{aligned} P[\text{forward jump} &= \tfrac{1}{2}(1 + Fx_j/2kT) \\ P[\text{reverse jump}] &= \tfrac{1}{2}(1 - Fx_j/2kT) \end{aligned} \tag{16}$$

The mean distance traveled in a jump is therefore given by

$$\begin{aligned} \mu &= \int \left\{ \frac{x_{j+1} + x_j}{2} \frac{1}{2}\left(1 + \frac{Fx_j}{2kT}\right) - \frac{x_{j-1} + x_j}{2} \frac{1}{2}\left(1 - \frac{Fx_j}{2kT}\right) \right\} \\ &\quad \times p(x_{j-1}, x_j, x_{j+1})\, dx_{j-1}\, dx_j\, dx_{j+1} \\ &= \frac{F}{4kT}(\langle x_j^2 \rangle + \langle x_j x_{j+1} \rangle) \end{aligned} \tag{17}$$

(clearly $\langle x_j x_{j+1} \rangle = \langle x_{j-1} x_j \rangle$).

In the absence of an applied field the probability of a forward jump is equal to that of a reverse jump. Thus

$$\begin{aligned} \sigma_0^2 &= \int \left[\frac{1}{2}\left(\frac{x_{j+1} + x_j}{2}\right)^2 + \frac{1}{2}\left(\frac{x_j + x_{j-1}}{2}\right)^2 \right] \\ &\quad \times p(x_{j-1}, x_j, x_{j+1})\, dx_{j-1}\, dx_j\, dx_{j+1} \\ &= \tfrac{1}{2}(\langle x_j^2 \rangle + \langle x_j x_{j+1} \rangle) \end{aligned} \tag{18}$$

Inserting these results into Eq. (14) shows that the Einstein relation is valid for all MW-type random walks corresponding to $1 < \nu < 2$.

For example, in Brownian motion Stokes' law is usually invoked to find K, e.g.,

$$F = 6\pi\eta a(\text{drift velocity}) \tag{19}$$

where η is the viscosity of the medium and a is the radius of the particle. We find that the usual formula

$$D = kT/6\pi\eta a \tag{20}$$

is valid even if the variance of the time interval between movements is infinite. This would correspond perhaps to a type of deep trapping; the effect of any trapping would be reflected in the value of η.

Consider now the case $0 < \nu < 1$ where a mean drift rate does not exist. We can define coefficients

$$D_e = \sigma_0^2/2\alpha \tag{21}$$

and

$$K_e = \mu/\alpha F \tag{22}$$

so that Eqs. (8) and (9) become

$$\langle x^2(t)\rangle = 2D_e t^\nu/\Gamma(1+\nu) \tag{23}$$

and

$$\langle x(t)\rangle = K_e F t^\nu/\Gamma(1+\nu) \tag{24}$$

However, the ratio D_e/K_e is independent of α, so that the same treatment as applied before to the Einstein relation is valid and

$$D_e/K_e = kT$$

Thus an observation of the drift behavior of particles [Eq. (24)] allows the pure diffusion behavior to be calculated [Eq. (23)]. The appropriate density for symmetric diffusion in Table I is also implied.

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