

ON THE MEAN SQUARE DISPLACEMENT IN LÉVY WALKS

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Abstract. Many physical and biological processes are modeled by “particles” undergoing Lévy random walks. A feature of significant interest in these systems is the mean square displacement (MSD) of the particles. Long-time asymptotic approximations of the MSD have been established, via the Tauberian Theorem, for systems in which the distribution of the step durations is asymptotically a power law of infinite variance. We extend these results, using elementary analysis, and obtain closed-form expressions as well as power law bounds for the MSD in equilibrium, and representations of the MSD as sums of super-linear, linear, and sub-linear terms. We show that the super-linear components are determined by the mean and asymptotics of the step durations, but that the linear and sub-linear components (whose size has implications for the accuracy of the asymptotic approximation) depend on the entire distribution function.

Key words. Lévy random walk, mean square displacement, super-diffusion, anomalous diffusion

AMS subject classifications. 60G51, 82C70

1. Introduction. We consider a random walker in \mathbb{R}^d moving at random velocities in straight line segments of random duration. At the end of each flight segment, a new velocity and duration are chosen at random. We assume that the durations and velocities are independent. Denote by F the distribution function of the duration. When F has infinite variance, the case of primary focus in this paper, this process is called a Lévy walk [20, 21, 25, 26, 30]. A swarm of random walkers starting at the same location and performing independent Lévy walks exhibits super-diffusion, that is, faster than linear growth in the *mean square displacement* (MSD) — the mean of the square of their distances from the origin. One finds many discussions of physical and biological applications of Lévy walks and related random processes leading to super-diffusion in the literature. Our own interest in the subject started when we modeled the evolution of a rarefied gas in an ultra-thin planar channel as a succession of infinite-variance flights and showed that the molecular density approaches a Gaussian distribution with a variance which grows super-linearly [5, 15, 23]. Other examples of applications include certain kinds of transport in fluid flow [26, 32], transport in biological cells [6, 28], the migration of bacteria [1], predator search behavior [27], and traveling humans [7]. Also, Lorentz gases [16, 33] and other billiards problems [2], in which there is no randomness in a strict sense but, rather, deterministic chaos, have been approximated by super-diffusive random walks.

The most commonly studied Lévy walks are those in which the speeds of the walkers are fixed. However, there are many interesting examples in which both the directions and the speeds of the flights are random [31]. For example, in the gas flow between horizontal plates with Maxwellian reflection conditions mentioned above, individual molecules undergo random flights whose durations and horizontal velocities are independent, with durations of infinite variance and finite expected square speed [5]. By allowing speeds to be random, but assuming that the expectation of the squared speed is finite, we include this and other examples without complicating the analysis beyond that of the single-speed case.

A fundamental quantity characterizing super-diffusion is the MSD. The common

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approach to analyzing the MSD is to formulate an equation describing the density of the walker location as a function of time and then to take a Fourier transform with respect to the space variables and a Laplace transform with respect to the time variable. One can then use the Tauberian theorem to deduce the long-time asymptotics of the MSD from the behavior of derivatives with respect to the Fourier variable near 0 [19, 21, 29].

An alternative and more elementary approach is to express the MSD as an integral over the velocity auto-correlation, and evaluate or analyze the integral; see for instance [2, 12]. We present a mathematical analysis of the basic properties of the MSD, using this approach, under the assumption that F has finite expectation.

While the standard approach is very useful in providing insights into various aspects of the *asymptotic* behavior of Lévy walks, the more elementary approach taken in this paper allows the derivation of *exact*, explicit expressions, valid for all times, for the MSD, for important classes of problems (Section 4). This enables detailed understanding of the accuracy of asymptotic approximations for the MSD (Section 6). In other examples, when exact expressions cannot be obtained, our approach permits the derivation of *time-dependent bounds*, valid for all times (Corollary 7.4).

We will distinguish between the “equilibrium” MSD, M_{eq} , and the “transitional” MSD, M_{tr} . Precise definitions are given in Section 2. The difference between the two cases lies in the interpretation of “ $t = 0$ ”. In the equilibrium case, $t = 0$ should be thought of as the time at which we start watching a random walk that has been going on for a long (strictly speaking, infinite) time. In the transitional case, the walk begins at time $t = 0$. The equilibrium case is easier to analyze since the MSD is then expressible as a simple convolution integral, and we focus on this case.

Long-time asymptotic approximations have been derived for various duration distributions, for both M_{tr} and M_{eq} . These approximations depend only on the tails of the distributions. However, accuracy of the asymptotic approximation may only emerge after an extremely long time. For instance, if M_{eq} is proportional to $t \log t$ to leading order, as occurs in numerous applications [2, 14, 33], there is typically a correction term of order t . For this term to become negligible, $1/\log t$ must become small, so t must be extremely large. We show that the presence or absence of a linear correction term depends on the entire distribution F , not just on its tail. Similarly we show that the presence of a logarithmic factor in $1 - F$ may cause M_{eq} to consist, to leading order, of a sum of two terms that only differ by a factor proportional to $\log t$. Highly precise and complete knowledge of F may therefore be needed to ascertain whether leading-order long-time asymptotic approximations for M_{eq} are accurate approximations to the actual M_{eq} at times of physical interest.

Of course, distributions found in real-world applications need not be exactly power laws asymptotically. We show that the model is robust in the sense that for distributions bounded by power laws, the MSDs also satisfy related bounds.

We relate the transitional MSD, M_{tr} , to the equilibrium MSD, M_{eq} . Our results on M_{tr} are weaker than those on M_{eq} and mostly concern the leading-order asymptotic behavior, but we also give a result on correction terms for M_{tr} . Finally, we present the asymptotic MSD for free molecular flow in planar channels [5].

2. Background and notation. Let T_i , $i = 0, 1, 2, \dots$, be random variables with

$$0 \leq T_0 < T_1 < T_2 < \dots$$

We will consider a random walker changing velocities at times T_i . We assume that the increments $\tau_i = T_i - T_{i-1}$, $i = 1, 2, 3, \dots$, are independent and identically distributed

positive random variables. The equilibrium and transitional cases differ in the choice of distribution of T_0 , as discussed below.

Let F denote the distribution of the τ_i . We assume throughout this paper that F is continuous and that its mean, $\bar{\tau}$, is finite:

$$\bar{\tau} = \int_0^\infty (1 - F(s)) ds < \infty.$$

Our primary concern in this paper is with the case when the second moment of F ,

$$\sigma^2 = \int_0^\infty 2s(1 - F(s)) ds, \quad (2.1)$$

is infinite.

At each time T_i a new velocity vector, V_i , is chosen. For simplicity of exposition, we will often refer to the times T_0, T_1, \dots as "collision" times, thinking of a particle colliding with a background. Thus the random selection of a new V_i is thought of as the result of a "collision". We assume that the velocities are identically distributed and independent of each other and of the collision times. We'll also assume that the mean velocity is zero, since if it were not, one could simply subtract the mean velocity and consider the shifted velocities (the only change would be a drift in the direction of the mean velocity). Denote by v the characteristic speed,

$$v = \sqrt{E[|V_i|^2]},$$

where $|\cdot|$ denotes the Euclidean norm. As we shall see below, given a duration distribution F , the MSD is proportional to $v^2 = E[|V_i|^2]$. This is the only dependence of the MSD on the velocity distribution. So, for example, given F , walks in d dimensions with post-collision velocities uniformly distributed on the sphere of radius v and those which go only in axial directions, with equal probabilities, at speed v , have identical MSDs — not just asymptotically, but for all time.

We consider two choices of T_0 :

1. *Transitional case*: $T_0 = 0$.
2. *Equilibrium case*: $T_0 > 0$ is random and independent of the τ_i , with distribution function

$$F_0(t) = \frac{1}{\bar{\tau}} \int_0^t (1 - F(s)) ds, \quad t > 0. \quad (2.2)$$

To review the significance of the distribution F_0 , recall [17] that for any $t \geq 0$,

$$Z_t = \min\{T_j : j \geq 0, T_j > t\} - t > 0$$

is called the *residual life at time t* . Denote its distribution function by $F_R(t, z)$, $z > 0$, so that for $t \geq 0$, $z > 0$,

$$F_R(t, z) = P(\exists j \geq 0 \quad t < T_j \leq t + z).$$

LEMMA 2.1. *If F is continuous, then $F_R(t, z)$ is a continuous function of $(t, z) \in [0, \infty) \times (0, \infty)$.*

Proof. Let $t \geq 0$, $z > 0$. Let Δt and Δz be numbers with $t + \Delta t \geq 0$ and $z + \Delta z > 0$. We must prove that $F_R(t + \Delta t, z + \Delta z) \rightarrow F_R(t, z)$ as $\Delta t, \Delta z \rightarrow 0$. We will consider the case $\Delta t \geq 0$ and $\Delta z \geq 0$. The cases when one or both of Δt and Δz are negative can be understood analogously.

We have

$$\begin{aligned} & \exists j \geq 0 \quad t + \Delta t < T_j \leq t + \Delta t + z + \Delta z \\ \Rightarrow & \exists j \geq 0 \quad t < T_j \leq t + \Delta t + z + \Delta z \\ \Rightarrow & \exists j \geq 0 \quad t < T_j \leq t + z \quad \text{or} \quad t + z < T_j \leq t + z + \Delta t + \Delta z \end{aligned}$$

and therefore

$$F_R(t + \Delta t, z + \Delta z) \leq F_R(t, z) + F_R(t + z, \Delta t + \Delta z). \quad (2.3)$$

Similarly,

$$\begin{aligned} & \exists j \geq 0 \quad t < T_j \leq t + z \\ \Rightarrow & \exists j \geq 0 \quad t < T_j \leq t + \Delta t + z + \Delta z \\ \Rightarrow & \exists j \geq 0 \quad t < T_j \leq t + \Delta t \quad \text{or} \quad t + \Delta t < T_j \leq t + \Delta t + z + \Delta z \end{aligned}$$

and therefore

$$F_R(t, z) \leq F_R(t, \Delta t) + F_R(t + \Delta t, z + \Delta z). \quad (2.4)$$

From (2.3) and (2.4),

$$|F_R(t + \Delta t, z + \Delta z) - F_R(t, z)| \leq \max(F_R(t + z, \Delta t + \Delta z), F_R(t, \Delta t)).$$

It therefore suffices to prove now that for any $a \geq 0$,

$$\lim_{\Delta t \rightarrow 0^+} P(\exists j \geq 0 \quad a < T_j \leq a + \Delta t) = 0. \quad (2.5)$$

To prove (2.5), we write, for any $n \geq 1$,

$$P(\exists j \geq 0 \quad a < T_j \leq a + \Delta t) \leq \sum_{j=1}^n P(a < T_j \leq a + \Delta t) + P(T_{n+1} \leq a + \Delta t). \quad (2.6)$$

Because F is continuous, the right-hand side of (2.6) converges to $P(T_{n+1} \leq a)$ as $\Delta t \rightarrow 0^+$. This implies

$$\limsup_{\Delta t \rightarrow 0^+} P(\exists j \geq 0 \quad a < T_j \leq a + \Delta t) \leq P(T_{n+1} \leq a).$$

The assertion now follows because $P(T_{n+1} \leq a) \rightarrow 0$ as $n \rightarrow \infty$. \square

The importance of F_0 lies in the following well-known result from renewal theory [17, Chapter XI, Section 4].

THEOREM 2.2. *In the equilibrium case,*

$$F_R(t, z) = F_0(z) \quad \text{for all } t \geq 0, z > 0.$$

In the transitional case,

$$\lim_{t \rightarrow \infty} F_R(t, z) = F_0(z) \quad \text{for all } z > 0.$$

We will use the following elementary fact.

LEMMA 2.3. *If $\sigma^2 < \infty$, then $1 - F(t) = o(1/t^2)$.*

Proof. Let τ denote a random variable with distribution function F . Let Ω denote the underlying probability space. For $t > 0$, let $I_t(\omega) = 1$ if $\tau(\omega) > t$, and $= 0$ otherwise. Then

$$t^2(1 - F(t)) = \int_{\tau(\omega) > t} t^2 d\omega \leq \int_{\tau(\omega) > t} \tau(\omega)^2 d\omega = \int_{\Omega} \tau(\omega)^2 I_t(\omega) d\omega.$$

The integrand converges to zero as $t \rightarrow \infty$ for any fixed ω , and is bounded by the integrable function $\tau(\omega)^2$. The Lebesgue dominated convergence theorem implies the assertion. \square

Some simple properties of F_0 that will be of use to us later on are collected in the following lemma.

LEMMA 2.4.

(a) *If F is continuous, then F_0 is continuously differentiable, with density*

$$\rho_0(t) = \frac{1 - F(t)}{\bar{\tau}}, \quad t > 0.$$

(b) *If $\sigma^2 < \infty$ then $1 - F_0(t) = o(1/t)$ as $t \rightarrow \infty$.*

(c) *The expectation of F_0 is $\sigma^2/(2\bar{\tau})$, regardless of whether σ^2 is finite or infinite.*

Proof. (a) follows from the fundamental theorem of calculus.

(b) Since $1 - F_0(t) = \frac{1}{\bar{\tau}} \int_t^\infty (1 - F(s)) ds$, this follows from Lemma 2.3.

(c) The expectation of F_0 is

$$\int_0^\infty (1 - F_0(s)) ds = [s(1 - F_0(s))]_0^\infty + \int_0^\infty s \frac{1 - F(s)}{\bar{\tau}} ds = \lim_{s \rightarrow \infty} s(1 - F_0(s)) + \frac{\sigma^2}{2\bar{\tau}}.$$

Using part (b), we see that this equals $\sigma^2/(2\bar{\tau})$. \square

Now define the random, piecewise constant velocity, V ,

$$V(t) = \begin{cases} V_0 & \text{if } 0 \leq t < T_0, \\ V_i & \text{if } T_{i-1} \leq t < T_i. \end{cases}$$

Consider a random walker in \mathbb{R}^d starting at $X(0) = 0$ and moving with velocity $V(t)$ at time t . The position of the random walker at time t is

$$X(t) = \int_0^t V(s) ds.$$

The *mean square displacement (MSD)* is the quantity

$$M(t) = E[|X(t)|^2].$$

As mentioned in the introduction, we use subscripts to distinguish the equilibrium and transitional cases, writing M_{eq} and M_{tr} and referring to M_{eq} as the *equilibrium MSD*, and to M_{tr} as the *transitional MSD*.

3. Integral representations and properties of the MSD.

3.1. The MSD as a double integral. The MSD can be expressed as an integral as follows [12]. For all $t \geq 0$,

$$\begin{aligned} M(t) &= E \left[\int_0^t V(r) dr \cdot \int_0^t V(s) ds \right] \\ &= E \left[\int_0^t \int_0^t V(r) \cdot V(s) dr ds \right] \\ &= 2E \left[\int_0^t \int_0^s V(r) \cdot V(s) dr ds \right]. \end{aligned}$$

Recalling that expectations are integrals over the sample space and using Fubini's theorem, we conclude that

$$M(t) = 2 \int_0^t \int_0^s E[V(r) \cdot V(s)] dr ds. \quad (3.1)$$

The auto-correlation $E[V(r) \cdot V(s)]$ that appears in (3.1) is related to the residual life distribution F_R as follows. Assume that $0 \leq r < s$. If there is no j with $T_j \in (r, s]$, an event of probability $1 - F_R(r, s - r)$, then $V(r) = V(s)$ and so $E[V(r) \cdot V(s)] = v^2$. If there is a j with $T_j \in (r, s]$, then $V(r)$ and $V(s)$ are independent and $E[V(r) \cdot V(s)] = 0$. Hence,

$$E[V(r) \cdot V(s)] = v^2 (1 - F_R(r, s - r)) \quad (3.2)$$

and, inserting (3.2) into (3.1),

$$M(t) = 2v^2 \int_0^t \int_0^s (1 - F_R(r, s - r)) dr ds \quad (3.3)$$

for all $t \geq 0$.

3.2. Properties of the MSD. We record the following general consequences of eq. (3.3).

PROPOSITION 3.1. *In both the equilibrium and transitional cases,*

- (a) $M(t) \sim v^2 t^2$ as $t \rightarrow 0$,
- (b) M is continuously differentiable,
- (c) $M'(t) > 0$ for all $t > 0$,
- (d) M grows at least linearly, i.e., $\liminf_{t \rightarrow \infty} M'(t) > 0$, and
- (e) for any fixed $s > 0$, $\lim_{t \rightarrow \infty} \frac{M(t-s)}{M(t)} = 1$.

Proof. (a) means

$$\frac{M(t)}{t^2} = \frac{2v^2}{t^2} \int_0^t \int_0^s (1 - F_R(r, s - r)) dr ds \rightarrow v^2,$$

and this holds because

$$\max \{F_R(r, s - r) : 0 \leq r < s \leq t\} \leq F(t) \rightarrow 0$$

as $t \rightarrow 0$. (b) follows immediately from (3.3) because F_R is a continuous function (Lemma 2.1). In fact,

$$M'(t) = 2v^2 \int_0^t (1 - F_R(r, t - r)) dr.$$

Note that $1 - F_R(r, t - r)$ is a non-negative continuous function of r and t which tends to 1 as $r \rightarrow t^-$. Thus, $M'(t) > 0$ for all $t > 0$, establishing (c). To prove (d), we will prove the existence of a positive lower bound on M' , valid for sufficiently large t . Let $a > 0$ and $t \geq a$. Then

$$\begin{aligned} M'(t) &= 2v^2 \int_0^t (1 - F_R(r, t - r)) dr \\ &\geq 2v^2 \int_{t-a}^t (1 - F_R(r, t - r)) dr \\ &\geq 2v^2 \int_{t-a}^t (1 - F_R(t - a, a)) dr \\ &= 2v^2 a (1 - F_R(t - a, a)) \\ &\rightarrow 2v^2 a (1 - F_0(a)) \end{aligned}$$

as $t \rightarrow \infty$. For sufficiently small $a > 0$, we have $2v^2 a (1 - F_0(a)) > 0$. Choose a so that this holds. Then for sufficiently large t ,

$$M'(t) \geq v^2 a (1 - F_0(a)) > 0.$$

This implies (d). To prove (e), first note $M(t) - M(t - s) > 0$ because of (c). Furthermore,

$$\begin{aligned} (M(t) - M(t - s))^2 &= (E[|X(t)|^2 - |X(t - s)|^2])^2 \\ &= (E[(|X(t)| - |X(t - s)|)(|X(t)| + |X(t - s)|)])^2 \\ &\leq E[|X(t) - X(t - s)|^2] E[|X(t) + X(t - s)|^2] \\ &\leq E\left[\left(\int_{t-s}^t |V(u)| du\right)^2\right] 2(E[|X(t)|^2] + E[|X(t - s)|^2]) \\ &\leq 2E\left[s \int_{t-s}^t |V(u)|^2 du\right] (E[|X(t)|^2] + E[|X(t - s)|^2]) \\ &= 2s \int_{t-s}^t E[|V(u)|^2] du (E[|X(t)|^2] + E[|X(t - s)|^2]) \\ &= 4v^2 s^2 M(t). \end{aligned}$$

Hence, $M(t) - M(t - s) \leq 2vs\sqrt{M(t)}$, and, since $M(t) \rightarrow \infty$ by (d), (e) follows. \square

3.3. Computing M_{eq} from F . As we have seen in Theorem 2.2, in the equilibrium case, $F_R(r, s - r) = F_0(s - r)$ for all r . Hence, eq. (3.3) becomes

$$M_{eq}(t) = 2v^2 \int_0^t \int_0^s (1 - F_0(s - r)) dr ds. \quad (3.4)$$

We now establish two consequences of this integral expression which will allow us both to construct illustrative examples and to establish the asymptotic behavior of the MSD. First, differentiating (3.4) and introducing the change of variables $t - r = u$, we find

$$M'_{eq}(t) = 2v^2 \int_0^t (1 - F_0(u)) du. \quad (3.5)$$

Equation (3.5) implies, by anti-differentiation, a representation of M_{eq} as a single integral:

$$M_{eq}(t) = 2v^2 \int_0^t (1 - F_0(u))(t - u) du. \quad (3.6)$$

Integrating by parts in (3.6), using (2.2), we obtain an integral expression for M_{eq} directly in terms of F rather than F_0 :

PROPOSITION 3.2. *For all $t \geq 0$, the equilibrium MSD can be expressed as*

$$\begin{aligned} M_{eq}(t) &= v^2 \left(t^2 - \frac{1}{\bar{\tau}} \int_0^t (1 - F(u))(t - u)^2 du \right) \\ &= \frac{v^2}{\bar{\tau}} \left(t^2 \int_t^\infty (1 - F(u)) du + \int_0^t (1 - F(u))(2tu - u^2) du \right). \end{aligned} \quad (3.7)$$

Proposition 3.2 will prove useful in deriving asymptotic results. We now derive an alternative characterization of M_{eq} , which will prove useful in constructing examples. Differentiating eq. (3.5), we obtain

$$M_{eq}''(t) = 2v^2(1 - F_0(t)). \quad (3.8)$$

Differentiating a third time, we arrive at the following proposition.

PROPOSITION 3.3. *M_{eq} is three times continuously differentiable and for all $t \geq 0$,*

$$M_{eq}'''(t) = \frac{2v^2}{\bar{\tau}}(F(t) - 1) \quad (3.9)$$

with boundary conditions,

$$M_{eq}(0) = 0, \quad M_{eq}'(0) = 0, \quad M_{eq}''(0) = 2v^2, \quad M_{eq}''(\infty) = 0. \quad (3.10)$$

It may appear at first sight that M_{eq} is over-determined by the four conditions in (3.10). However, note that (3.9) implies that $M_{eq}''(0) - M_{eq}''(\infty) = 2v^2$. Therefore, $M_{eq}''(0) = 2v^2$ and $M_{eq}''(\infty) = 0$ are equivalent conditions.

4. A family of power laws with closed-form M_{eq} . A standard assumption in the literature is that F is, asymptotically, a power law. This enables derivation of asymptotic behavior of Lévy walks, including the MSD, via Laplace transforms and the Tauberian theorem [21].

However, in the equilibrium case, for a variety of power laws, one can get a more precise result — the exact MSD for all times. For example, for $\alpha > 1$ and $t_0 > 0$, let

$$F(t) = 1 - \left(1 + \frac{t}{t_0}\right)^{-\alpha}. \quad (4.1)$$

The mean of this distribution is

$$\bar{\tau} = \int_0^\infty \left(1 + \frac{t}{t_0}\right)^{-\alpha} dt = \frac{t_0}{\alpha - 1}. \quad (4.2)$$

For $\alpha \leq 2$, the second moment of F is infinite, while for $\alpha > 2$, it is finite. Using (4.2), we see that in the limit as $\alpha \rightarrow \infty$, with $\bar{\tau}$ fixed, we obtain the exponential distribution

$$F(t) = 1 - e^{-t/\bar{\tau}}. \quad (4.3)$$

We also note that

$$F_0(t) = \frac{1}{\bar{\tau}} \int_0^t (1 - F(s)) ds = 1 - \left(1 + \frac{t}{t_0}\right)^{1-\alpha}.$$

Using either Proposition 3.2 or Proposition 3.3, we can compute $M_{eq}(t)$ exactly for the distributions in (4.1) and (4.3). For example, consider the case $\alpha = 3$. Using eqs. (3.9) and (4.2), we obtain

$$M_{eq}'''(t) = \frac{4v^2}{t_0} \left(1 + \frac{t}{t_0}\right)^{-3}.$$

Integrating, using the boundary conditions (3.10), we find

$$M_{eq}''(t) = -2v^2 \left(1 + \frac{t}{t_0}\right)^{-2},$$

$$M_{eq}'(t) = 2v^2 t_0 - 2v^2 t_0 \left(1 + \frac{t}{t_0}\right)^{-1},$$

and

$$M_{eq}(t) = 2v^2 t_0^2 \left(\frac{t}{t_0} - \log \left(1 + \frac{t}{t_0}\right) \right).$$

This proves eq. (4.6) below. The other parts of Proposition 4.1 are proved by similar straightforward calculations.

PROPOSITION 4.1. *For the distribution given by (4.1) if $\alpha < \infty$, and by (4.3) if $\alpha = \infty$, we have, for all $t \geq 0$,*

$$M_{eq}(t) = \begin{cases} \frac{2(vt_0)^2}{(2-\alpha)(3-\alpha)} \left(\left(1 + \frac{t}{t_0}\right)^{3-\alpha} - (3-\alpha) \frac{t}{t_0} - 1 \right) & \text{if } \alpha > 1, \alpha \neq 2, 3 \quad (4.4) \\ 2(vt_0)^2 \left(\left(1 + \frac{t}{t_0}\right) \log \left(1 + \frac{t}{t_0}\right) - \frac{t}{t_0} \right) & \text{if } \alpha = 2 \quad (4.5) \\ 2(vt_0)^2 \left(\frac{t}{t_0} - \log \left(1 + \frac{t}{t_0}\right) \right) & \text{if } \alpha = 3 \quad (4.6) \\ 2(v\bar{\tau})^2 \left(\frac{t}{\bar{\tau}} - 1 + e^{-t/\bar{\tau}} \right) & \text{if } \alpha = \infty \quad (4.7) \end{cases}$$

We stress again that these are *exact* formulas valid for all times, not just *asymptotic* ones. Note that (4.4) tends to (4.5) as $\alpha \rightarrow 2$, and to (4.6) as $\alpha \rightarrow 3$. Using (4.2), it is also straightforward to see that in the limit as $\alpha \rightarrow \infty$ with $\bar{\tau}$ fixed, (4.4) tends to (4.7).

When the particles move at a constant speed v , there is a sharp front consisting of particles which have experienced no collisions. Then at time t , the probability of having experienced no collisions is $1 - F_0(t)$ and the contribution to M_{eq} of this front is $v^2 t^2 (1 - F_0(t))$. For the above power law with $1 < \alpha < 2$, this gives a contribution of

$$M_{eq}^f(t) = v^2 t^2 \left(1 + \frac{t}{t_0}\right)^{1-\alpha}.$$

As $t \rightarrow \infty$, the front contributes an asymptotically constant proportion to the total MSD:

$$\frac{M_{eq}^f(t)}{M_{eq}(t)} \rightarrow \frac{(2-\alpha)(3-\alpha)}{2}.$$

For $\alpha \geq 2$, the contribution of the front to $M_{eq}(t)$ becomes negligible as $t \rightarrow \infty$.

5. Leading-order asymptotics of M_{eq} . If F has finite variance, then

$$\lim_{t \rightarrow \infty} M'_{eq}(t) = 2v^2 \lim_{t \rightarrow \infty} \int_0^t (1 - F_0(s)) ds = \frac{\sigma^2 v^2}{\bar{\tau}},$$

by eq. (3.5) together with Lemma 2.4, part (c). Hence,

$$M_{eq}(t) \sim \sigma^2 v^2 \frac{t}{\bar{\tau}} \quad \text{as } t \rightarrow \infty. \quad (5.1)$$

The more interesting case is that of infinite variance, to which we now turn. In several places we will make use of the following lemma.

LEMMA 5.1. *Let f and g be non-negative, locally integrable functions of $t \in [0, \infty)$ with $f(t) > 0$ and $g(t) > 0$ for sufficiently large t ,*

$$f(t) \sim g(t) \quad \text{as } t \rightarrow \infty,$$

and

$$\int_0^\infty f(t) dt = \int_0^\infty g(t) dt = \infty.$$

Then

$$\int_0^t f(s) ds \sim \int_0^t g(s) ds \quad \text{as } t \rightarrow \infty.$$

Proof. Let $\epsilon > 0$. Choose $A > 0$ so that for $t \geq A$, $f(t) \leq (1 + \epsilon)g(t)$. Then for $t \geq A$,

$$\begin{aligned} \int_0^t f(s) ds &= \int_0^A f(s) ds + \int_A^t f(s) ds \leq \int_0^A f(s) ds + (1 + \epsilon) \int_A^t g(s) ds \\ &\leq \int_0^A f(s) ds + (1 + \epsilon) \int_0^t g(s) ds. \end{aligned}$$

Therefore

$$\frac{\int_0^t f(s) ds}{\int_0^t g(s) ds} \leq \frac{\int_0^A f(s) ds}{\int_0^t g(s) ds} + 1 + \epsilon.$$

Letting $t \rightarrow \infty$, we find

$$\limsup_{t \rightarrow \infty} \frac{\int_0^t f(s) ds}{\int_0^t g(s) ds} \leq 1 + \epsilon.$$

By a similar argument,

$$\liminf_{t \rightarrow \infty} \frac{\int_0^t f(s) ds}{\int_0^t g(s) ds} \geq 1 - \epsilon.$$

Since these conclusions hold for any $\epsilon > 0$, the assertion follows. \square

The following theorem shows that in the infinite variance case, the leading-order long-time asymptotic behavior of $\bar{\tau}M_{eq}$ is determined by the leading-order long-time asymptotic behavior of $1 - F$.

THEOREM 5.2. *Let F and \tilde{F} be infinite-variance distributions with finite means $\bar{\tau}$ and $\tilde{\tau}$ and equilibrium MSDs M_{eq} and \tilde{M}_{eq} , respectively. Assume that*

$$1 - F(t) \sim 1 - \tilde{F}(t) \quad \text{as } t \rightarrow \infty.$$

Then

$$\bar{\tau}M_{eq}(t) \sim \tilde{\tau}\tilde{M}_{eq}(t) \quad \text{as } t \rightarrow \infty.$$

Proof. $\bar{\tau}M_{eq}''' = 2v^2(F-1)$, $M_{eq}''(\infty) = 0$ and $\tilde{\tau}\tilde{M}_{eq}''' = 2v^2(\tilde{F}-1)$, $\tilde{M}_{eq}''(\infty) = 0$ imply

$$\bar{\tau}M_{eq}''(t) = \int_t^\infty 2v^2(1 - F(s)) ds \sim \tilde{\tau}\tilde{M}_{eq}''(t) = \int_t^\infty 2v^2(1 - \tilde{F}(s)) ds$$

as $t \rightarrow \infty$. From Lemma 2.4, part (c), and eq. (3.5), we know that $M'_{eq}(t)$ and $\tilde{M}'_{eq}(t)$ tend to ∞ as $t \rightarrow \infty$. This implies, using Lemma 5.1, that

$$\bar{\tau}M'_{eq}(t) = \int_0^t \bar{\tau}M_{eq}''(s)ds \sim \tilde{\tau}\tilde{M}'_{eq}(t) = \int_0^t \tilde{\tau}\tilde{M}_{eq}''(s)ds.$$

Because $M_{eq}(t)$ and $\tilde{M}_{eq}(t)$ tend to ∞ , this in turn implies, again by Lemma 5.1,

$$\bar{\tau}M_{eq}(t) = \int_0^t \bar{\tau}M'_{eq}(s)ds \sim \tilde{\tau}\tilde{M}_{eq}(t) = \int_0^t \tilde{\tau}\tilde{M}'_{eq}(s)ds,$$

which is the statement of the theorem. \square

Proposition 4.1 and Theorem 5.2 together imply the well-known formulas [3, 24] for the leading-order asymptotic behavior of M_{eq} for $\alpha \in (1, 2]$, summarized in the following corollary. We add to the statement of this corollary the result for the finite variance case $\alpha > 2$ (see eq. (5.1)).

COROLLARY 5.3. *Suppose that*

$$1 - F(t) \sim \left(\frac{t}{t_0}\right)^{-\alpha}$$

for some $t_0 > 0$ and $\alpha > 1$. Then as $t \rightarrow \infty$,

$$M_{eq}(t) \sim \begin{cases} \frac{t_0}{\bar{\tau}} \frac{2(vt_0)^2}{(\alpha-1)(2-\alpha)(3-\alpha)} \left(\frac{t}{t_0}\right)^{3-\alpha} & \text{if } 1 < \alpha < 2, \\ \frac{t_0}{\bar{\tau}} 2(vt_0)^2 \frac{t}{t_0} \log \frac{t}{t_0} & \text{if } \alpha = 2, \\ \frac{t_0}{\bar{\tau}} (v\sigma)^2 \frac{t}{t_0} & \text{if } \alpha > 2. \end{cases} \quad (5.2)$$

$$(5.2)$$

$$(5.3)$$

$$(5.4)$$

6. Accuracy of leading-order asymptotics: Examples.. In this section we explore the accuracy of leading-order asymptotic descriptions of M_{eq} such as those given in Corollary 5.3.

6.1. Canonical power laws. For the power laws

$$F(t) = 1 - \left(1 + \frac{t}{t_0}\right)^{-\alpha}$$

discussed in Section 4, the accuracy of the leading-order asymptotics can be ascertained from eqs. (4.4)–(4.6). The discrepancy between the exact M_{eq} and the leading-order asymptotics given in Corollary 5.3 is $O(t/t_0)$ for $\alpha \leq 2$, and $O((t/t_0)^{3-\alpha})$ for $2 < \alpha < 3$. Therefore the leading-order asymptotic approximation for $M_{eq}(t)$ is inaccurate when $\alpha \approx 2$ unless t/t_0 is very large.

Figure 6.1 illustrates this conclusion, using $t_0 = 1$, $v = 1$, and six different values of α . The figure shows, for $0 \leq t \leq 1000$, the exact $M_{eq}(t)$ (solid), the leading-order approximations (dotted), and Monte Carlo estimates of M_{eq} (circles), based on 500,000 simulated random walkers for each value of α .

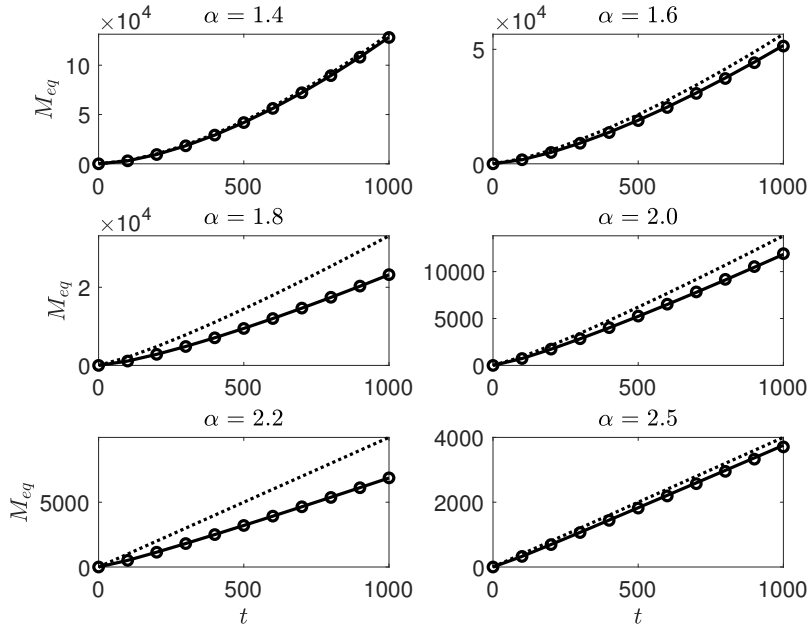


Fig. 6.1: Exact M_{eq} (solid), leading-order approximation as given in Corollary 5.3 (dotted), and approximations of M_{eq} obtained by simulations of 500,000 walkers (circles) for six different values of α .

For $\alpha = 2$, the relative difference between M_{eq} and its leading-order approximation is approximately $1/\log(t/t_0)$, and for this to be smaller than 0.05, corresponding to 5% accuracy, we need $t/t_0 > e^{20} \approx 5 \times 10^8$. Zarfaty et al. [33] relate slow convergence of M_{eq} to slow convergence in the Central Limit Theorem (CLT) for $\alpha = 2$ [22], a special case of slow convergence for any slowly varying scaling in the generalized CLT [4]. A related, deterministic, problem is that of infinite-horizon billiards, in which the asymptotic MSD also contains a logarithmic factor. For this case, Cristadoro

et al. derived the first two terms in the asymptotic expansion of the MSD [9] and demonstrated numerically that the leading-order term is a poor approximation of the actual MSD for reasonable lengths of time [10]. In [11], the same authors derived an evolution equation for the MSD for random walks on a lattice with exponentially distributed waiting times between flight segments, a problem that can be seen as an abstraction of the infinite-horizon Lorentz gas when $\alpha = 2$.

6.2. A general approach to constructing examples. Instead of beginning with F and computing M_{eq} , we can also, for the purposes of constructing interesting examples, start with M_{eq} and compute F from it, based on the following proposition.

PROPOSITION 6.1. *Let $\mathcal{M} \in C^3([0, \infty))$. There exist an expected speed $v > 0$ and a continuous probability distribution function F on $(0, \infty)$ with finite mean $\bar{\tau}$ such that $M_{eq} = \mathcal{M}$ is the equilibrium MSD associated with v and F if and only if*

1. $\mathcal{M}(0) = \mathcal{M}'(0) = 0$,
2. $\mathcal{M}''(0) > 0$ and $\mathcal{M}''(\infty) = 0$,
3. \mathcal{M}''' is an increasing function with $\mathcal{M}'''(0) < 0$ and $\mathcal{M}'''(\infty) = 0$.

In that case,

$$v^2 = \frac{\mathcal{M}''(0)}{2}, \quad F(t) = 1 - \frac{\mathcal{M}'''(t)}{\mathcal{M}'''(0)}, \quad \bar{\tau} = \frac{\mathcal{M}''(0)}{|\mathcal{M}'''(0)|}.$$

Proof. This is a straightforward consequence of Proposition 3.3. \square

6.3. Accurate leading-order asymptotics. Examples in which there are accurate leading-order asymptotic descriptions of M_{eq} can be constructed using Proposition 6.1. For instance,

$$M_{eq} = v^2 t \log(1+t) = v^2 t \log t + O(1)$$

when

$$F(t) = 1 - \frac{3+t}{3(1+t)^3},$$

and for $1 < \alpha < 2$,

$$M_{eq}(t) = v^2 t^2 (1+t)^{1-\alpha} = v^2 t^{3-\alpha} + O(t^{2-\alpha})$$

when

$$F(t) = 1 - (1+t)^{-\alpha} \left(1 - \frac{\alpha t}{1+t} + \frac{\alpha(\alpha+1)t^2}{6(1+t)^2} \right).$$

6.4. Logarithmic factors for $\alpha \in (1, 2)$. What happens when the distribution function is asymptotically close to, but not exactly, a power law? For example, set

$$F(t) = 1 - \frac{1 + \log(1+t)}{(1+t)^{3/2}}.$$

A closed-form equilibrium MSD can be derived for this distribution function, as well:

$$\begin{aligned} M_{eq}(t) &= v^2 \left(\frac{8}{9} (t+1)^{3/2} \log(t+1) + \frac{8}{27} (t+1)^{3/2} - \frac{4}{3} t - \frac{8}{27} \right) \\ &= v^2 \frac{8}{9} t^{3/2} \left(\log(t) + \frac{1}{3} \right) + O(t). \end{aligned}$$

The leading-order approximation $M_{eq}(t) \sim v^2 \frac{8}{9} t^{3/2} \log t$ is very poor because the next-most-significant term is $O(t^{3/2})$.

7. Super-linear, linear, and sub-linear terms. We saw in the last section that linear correction terms can have considerable implications for the accuracy of the leading-order approximation of M_{eq} when α is near 2. Here we show that for $\alpha \in (1, 2]$, the linear contributions to M_{eq} depend on the entire distribution F , while super-linear terms, for a given $\bar{\tau}$, only depend on the asymptotic behavior of F .

The following theorem shows that the entire distribution F is needed to compute linear contributions to M_{eq} : The value of $\bar{\tau}$ and the precise tail of F (i.e., $F(t)$ for $t \geq A$, for some $A > 0$) do not determine the linear contributions.

THEOREM 7.1. *Let F be continuously differentiable, with equilibrium MSD M_{eq} . Then for all $A > 0$ such that $F(A) > 0$, there exists a distribution function \tilde{F} , with equilibrium MSD \tilde{M}_{eq} , such that the means of F and \tilde{F} agree, F and \tilde{F} agree on $[A, \infty)$, and*

$$|M_{eq}(t) - \tilde{M}_{eq}(t)| \geq O(t)$$

as $t \rightarrow \infty$.

Proof. By eq. (3.7), if F and \tilde{F} agree on $[A, \infty)$, then for all $t \geq A$,

$$M_{eq}(t) - \tilde{M}_{eq}(t) = -\frac{v^2}{\bar{\tau}} \int_0^A (F(u) - \tilde{F}(u))(2tu - u^2) du.$$

Hence, to complete the proof, it suffices to find an increasing \tilde{F} such that

$$\int_0^A (F(u) - \tilde{F}(u)) du = 0 \quad \text{but} \quad \int_0^A (F(u) - \tilde{F}(u)) u du \neq 0,$$

which is, of course, always possible. \square

On the other hand, the following theorem shows that the value of $\bar{\tau}$ and knowledge of F up to a "finite variance" piece are sufficient to determine super-linear contributions to M_{eq} .

THEOREM 7.2. *Let*

$$1 - F(t) = G(t) + H(t),$$

where G and H are integrable functions of $t > 0$ with

$$\int_0^\infty |H(t)| t dt < \infty. \quad (7.1)$$

Then

$$M_{eq}(t) = \frac{v^2}{\bar{\tau}} \left(t^2 \int_t^\infty G(u) du + \int_0^t G(u)(2tu - u^2) du \right) + O(t). \quad (7.2)$$

Assumption (7.1) makes precise the assertion that H is a "finite variance piece"; compare eq. (2.1).

Proof. Because of Proposition 3.2 and assumption (7.1), it is enough to prove

$$\left| \int_t^\infty H(u) du \right| = O\left(\frac{1}{t}\right) \quad \text{and} \quad \left| \int_0^t H(u) u^2 du \right| = O(t).$$

Both follow from (7.1):

$$\left| \int_t^\infty H(u) du \right| \leq \int_t^\infty |H(u)| u \frac{1}{u} du \leq \int_t^\infty |H(u)| u du \frac{1}{t} = o\left(\frac{1}{t}\right)$$

and

$$\left| \int_0^t H(u) u^2 du \right| \leq \int_0^t |H(u)| u du \leq \int_0^\infty |H(u)| u du = O(t).$$

□

In particular, this proposition implies that an asymptotic expansion of the slowly converging part of $1 - F$ translates into an asymptotic expansion of the super-linear part of M_{eq} :

COROLLARY 7.3. *Suppose that*

$$1 - F(t) = \sum_{j=1}^n C_j t^{-p_j} + Ct^{-2} + O(t^{-q}) \quad (7.3)$$

as $t \rightarrow \infty$, where $n \geq 0$,

$$1 < p_1 < \dots < p_n < 2, \quad q > 2,$$

and the C_j and C are constants. Then

$$M_{eq}(t) = \frac{2v^2}{\bar{\tau}} \left[\sum_{j=1}^n \frac{C_j}{(p_j - 1)(2 - p_j)(3 - p_j)} t^{3-p_j} + Ct \log t \right] + O(t). \quad (7.4)$$

Proof. We set

$$G(t) = \begin{cases} \sum_{j=1}^n C_j t^{-p_j} + Ct^{-2} & \text{for } t \geq 1, \\ 0 & \text{for } t < 1, \end{cases}$$

and

$$H(t) = 1 - F(t) - G(t) = O(t^{-q}).$$

Theorem 7.2 implies that

$$\begin{aligned} M_{eq}(t) &= \frac{v^2}{\bar{\tau}} \left[t^2 \int_t^\infty \left(\sum_{j=1}^n C_j u^{-p_j} + Cu^{-2} \right) du + 2t \int_1^t \left(\sum_{j=1}^n C_j u^{-p_j} + Cu^{-2} \right) u du \right. \\ &\quad \left. - \int_1^t \left(\sum_{j=1}^n C_j u^{-p_j} + Cu^{-2} \right) u^2 du \right] + O(t). \end{aligned}$$

The assertion follows by evaluating the integrals. □

What happens if F doesn't follow a power law exactly? Power law bounds on F give us bounds on the MSD. For instance, we have the following result.

COROLLARY 7.4.

(a) Let $\alpha \in (1, 2)$, $C > 0$. If

$$1 - F(t) \leq Ct^{-\alpha}$$

for all $t > 0$, then

$$M_{eq}(t) \leq \frac{2v^2}{\bar{\tau}} \frac{C}{(\alpha - 1)(2 - \alpha)(3 - \alpha)} t^{3-\alpha}$$

for all $t > 0$. Similarly, if $1 - F(t) \geq Ct^{-\alpha}$ for all $t > 0$, then the reverse inequality holds.

(b) Let $C > 0$ and $A > 0$. If

$$1 - F(t) \leq Ct^{-2}$$

for all $t \geq A$, then

$$M_{eq}(t) \leq \frac{v^2}{\bar{\tau}} \left[CA + \int_0^A (1 - F(u))(2tu - u^2) du + 2Ct \log \frac{t}{A} \right]$$

for $t \geq A$. Similarly, if $1 - F(t) \geq Ct^{-2}$ for all $t \geq A$, then the reverse inequality holds.

Proof. These are immediate consequences of Proposition 3.2. \square

8. Asymptotic behavior of M_{tr} . We next relate M_{eq} and M_{tr} to each other, in order to deduce asymptotic behavior of M_{tr} from the asymptotic behavior of M_{eq} . (See also [3], where expressions for M_{eq} and M_{tr} are obtained from assumed forms of the Laplace transform of the duration density in a more general setting.) Let $t > 0$ and denote by X_{eq} the position of the equilibrium process. Then the conditional expectation of $X_{eq}(t)^2$, given that $T_0 > t$, is $(vt)^2$. If $T_0 \leq t$, then $X_{eq}(t)$ consists of the initial segment of duration T_0 , and the rest. The displacements experienced in these two segments are not independent — when T_0 is larger, the second segment is briefer. They are, however, uncorrelated, and therefore the variances of the displacements add. Writing as before $\rho_0 = F'_0 = (1 - F)/\bar{\tau}$, we have

$$M_{eq}(t) = (1 - F_0(t))(vt)^2 + \int_0^t \rho_0(s)((vs)^2 + M_{tr}(t - s)) ds. \quad (8.1)$$

Equation (8.1) can be read as an equation representing $\rho_0 * M_{tr}$ in terms of M_{eq} :

$$(\rho_0 * M_{tr})(t) = M_{eq}(t) - (1 - F_0(t))(vt)^2 - \int_0^t \rho_0(s)(vs)^2 ds.$$

By integration by parts, this can be re-written more simply:

$$(\rho_0 * M_{tr})(t) = M_{eq}(t) - 2v^2 \int_0^t (1 - F_0(s)) s ds. \quad (8.2)$$

LEMMA 8.1.

$$\rho_0 * M_{tr}(t) \sim M_{tr}(t) \quad \text{as } t \rightarrow \infty.$$

Proof. It is clear that

$$\rho_0 * M_{tr}(t) = \int_0^t \rho_0(s) M_{tr}(t - s) ds \leq M_{tr}(t)$$

for all t , since M_{tr} is strictly increasing (Proposition 3.1, part (c)). Now let $\epsilon > 0$. Let S be so large that

$$\int_0^S \rho_0(s) ds \geq 1 - \epsilon.$$

Then for $t \geq S$,

$$\rho_0 * M_{tr}(t) = \int_0^t \rho_0(s) M_{tr}(t - s) ds \geq \int_0^S \rho_0(s) M_{tr}(t - s) ds \geq (1 - \epsilon) M_{tr}(t - S).$$

For t sufficiently large, this is $\geq (1 - \epsilon)^2 M_{tr}(t)$ since $M_{tr}(t - S) \sim M_{tr}(t)$ as $t \rightarrow \infty$ (Proposition 3.1, part (e)). Since the above arguments hold for all $\epsilon > 0$, the assertion follows. \square

THEOREM 8.2. *If $\sigma^2 < \infty$, then*

$$M_{tr}(t) \sim M_{eq}(t) \sim \sigma^2 v^2 \frac{t}{\bar{\tau}}$$

as $t \rightarrow \infty$.

Proof. This follows from eq. (8.2), together with Lemma 8.1, Lemma 2.4, part (b), and eq. (5.1). \square

For power laws with exponent $\alpha \in (1, 2)$, the smaller $\alpha - 1$ (and hence the greater the first step of the equilibrium process), the more we might expect M_{eq} to exceed M_{tr} . For fixed α , the two MSDs are asymptotically proportional, but, indeed, the asymptotic ratio of M_{tr} to M_{eq} is $\alpha - 1$, as seen in [3, 13, 18].

THEOREM 8.3. *Let*

$$1 - F(t) \sim \left(\frac{t}{t_0}\right)^{-\alpha} \quad (8.3)$$

as $t \rightarrow \infty$, for some constant $t_0 > 0$. Then

(a) $M_{tr} \sim (\alpha - 1)M_{eq}$ if $\alpha \in (1, 2)$, and

(b) $M_{tr} \sim M_{eq}$ if $\alpha \geq 2$.

Proof. (a) Let $\alpha \in (1, 2)$. From (8.3),

$$1 - F_0(t) = \frac{1}{\bar{\tau}} \int_t^\infty (1 - F(s)) ds \sim \frac{t_0}{\bar{\tau}(\alpha - 1)} \left(\frac{t}{t_0}\right)^{-\alpha+1}.$$

This yields, using Lemma 5.1, the asymptotic behavior of the second term on the right-hand side of eq. (8.2):

$$2v^2 \int_0^t (1 - F_0(s)) s ds \sim \frac{2t_0(vt_0)^2}{\bar{\tau}(\alpha - 1)(3 - \alpha)} \left(\frac{t}{t_0}\right)^{3-\alpha}.$$

From eq. (4.4) and Theorem 5.2,

$$M_{eq}(t) \sim \frac{t_0/(\alpha - 1)}{\bar{\tau}} \frac{2(vt_0)^2}{(2 - \alpha)(3 - \alpha)} \left(\frac{t}{t_0}\right)^{3-\alpha}.$$

Therefore, by eq. (8.2) and Lemma 8.1,

$$M_{tr} \sim \frac{t_0}{\bar{\tau}} \frac{2(vt_0)^2}{(\alpha - 1)(2 - \alpha)(3 - \alpha)} \left(\frac{t}{t_0}\right)^{3-\alpha} - \frac{t_0}{\bar{\tau}} \frac{2(vt_0)^2}{(\alpha - 1)(3 - \alpha)} \left(\frac{t}{t_0}\right)^{3-\alpha} \sim (\alpha - 1)M_{eq}.$$

(b) For $\alpha > 2$, we have $\sigma^2 < \infty$, and therefore the assertion follows from Theorem 8.2. For $\alpha = 2$,

$$1 - F_0(t) = \frac{1}{\bar{\tau}} \int_t^\infty (1 - F(s)) ds \sim \frac{t_0^2}{\bar{\tau}t}$$

and therefore, using Lemma 5.1,

$$2v^2 \int_0^t (1 - F_0(s)) s ds \sim 2(vt_0)^2 \frac{t}{\bar{\tau}}. \quad (8.4)$$

By eq. (4.5) and Theorem 5.2,

$$M_{eq}(t) \sim 2(vt_0)^2 \frac{t}{\bar{\tau}} \log \frac{t}{t_0}.$$

Therefore, by eq. (8.2) and Lemma 8.1, $M_{tr}(t) \sim M_{eq}(t)$. \square

For specific examples, (8.2) enables us to compute $\rho_0 * M_{tr}$, but not M_{tr} . We know from Lemma 8.1 that the leading-order asymptotic behavior of $\rho_0 * M_{tr}$ is the same as that of M_{tr} . However, in special cases, knowledge of $\rho_0 * M_{tr}$ yields more than just the leading-order asymptotic behavior. We give the following example.

LEMMA 8.4. *Assume that*

$$1 - F(t) \sim \left(\frac{t}{t_0}\right)^{-2} \quad \text{as } t \rightarrow \infty,$$

for some $t_0 > 0$. Then there exists a constant $C > 0$ such that for all sufficiently large t ,

$$0 \leq M_{tr}(t) - \rho_0 * M_{tr}(t) \leq C\sqrt{t(\log t)^3}.$$

Proof. We noted in the proof of Lemma 8.1 that $\rho_0 * M_{tr}(t)$ is a lower bound on $M_{tr}(t)$, so $0 \leq M_{tr}(t) - \rho_0 * M_{tr}(t)$. We will now find an upper bound on $M_{tr}(t) - \rho_0 * M_{tr}(t)$:

$$\begin{aligned} M_{tr}(t) - \rho_0 * M_{tr}(t) &= \int_0^\infty \rho_0(s) M_{tr}(t) ds - \int_0^t \rho_0(s) M_{tr}(t-s) ds \\ &= \int_0^t \rho_0(s) (M_{tr}(t) - M_{tr}(t-s)) ds + \int_t^\infty \rho_0(s) ds M_{tr}(t). \end{aligned} \quad (8.5)$$

In the proof of Proposition 3.1, we saw:

$$M_{tr}(t) - M_{tr}(t-s) < 2vs \sqrt{M_{tr}(t)}.$$

Using this in (8.5), we find the upper bound

$$2v\sqrt{M_{tr}(t)} \int_0^t s \rho_0(s) ds + \int_t^\infty \rho_0(s) ds M_{tr}(t) \quad (8.6)$$

By hypothesis,

$$\rho_0(t) \sim \frac{1}{\bar{\tau}} \left(\frac{t}{t_0}\right)^{-2} \quad (8.7)$$

as $t \rightarrow \infty$. This implies

$$\int_0^t s \rho_0(s) ds \sim \frac{t_0^2}{\bar{\tau}} \log t. \quad (8.8)$$

We know from Theorem 8.3 that

$$M_{tr}(t) \sim C_1 t \log t \quad (8.9)$$

for some positive constant C_1 . Furthermore, from (8.7),

$$\int_t^\infty \rho_0(s) ds \sim \frac{t_0^2}{\bar{\tau}} t^{-1}. \quad (8.10)$$

Using (8.8)–(8.10) in (8.6), we obtain the assertion. \square

As was the case for equilibrium Lévy walks, even exact knowledge of the tails and means of step durations doesn't suffice to determine the linear terms of the asymptotics of the transitional MSDs:

THEOREM 8.5. *Let a distribution F , with mean $\bar{\tau}$, satisfy*

$$1 - F(t) \sim \left(\frac{t}{t_0}\right)^{-2}$$

as $t \rightarrow \infty$, for some $t_0 > 0$, and let $A > 0$ be given. Then there exists a distribution \tilde{F} with the same mean, $\bar{\tau}$, and with

$$F(t) = \tilde{F}(t) \quad \text{for all } t \geq A,$$

such that the corresponding mean square displacements M_{tr} and \tilde{M}_{tr} differ by at least $O(t)$.

Proof. Let \tilde{F} be as in Theorem 7.1. By Lemma 8.4 and eqs. (8.2) and (8.4),

$$M_{tr}(t) = M_{eq}(t) - 2(vt_0)^2 \frac{t}{\bar{\tau}} + o(t),$$

and similarly

$$\tilde{M}_{tr}(t) = \tilde{M}_{eq}(t) - 2(vt_0)^2 \frac{t}{\bar{\tau}} + o(t),$$

as $t \rightarrow \infty$. Since, by Theorem 7.1, $M_{eq}(t)$ and $\tilde{M}_{eq}(t)$ differ by $\geq O(t)$, so do M_{tr} and \tilde{M}_{tr} . \square

For the canonical power laws of Section 6.1, Figure 8.1 illustrates our results by showing, for six different values of α , the exact MSD (solid) and the leading order asymptotic approximation (dots) for the equilibrium (black) and transitional (dots) cases.

9. Application to free molecular flow in a planar channel. We studied the flow of a rarefied gas in an infinite planar channel in [5]. Assuming that length units are chosen so that the thickness of the channel is 1, we take the flow domain to be

$$\{(x_1, x_2, z) \in \mathbb{R}^3 : 0 < z < 1\}.$$

We refer to $x = (x_1, x_2)$ as the “horizontal” coordinates, and to z as the “vertical” coordinate. As in [5], we consider the projection of a particle trajectory into the (x_1, x_2) -plane. Gas molecules are assumed not to interact with each other, to travel at constant velocities in the interior of the channel, and to undergo random reflections at the walls, described by Maxwell's boundary conditions [8, pp. 118 ff] (the accommodation coefficient in [5] is arbitrary, but we take it to be 1 here for simplicity). Specifically, a gas molecule that hits the lower wall $z = 0$ re-emerges with a random velocity (V, W) , $V \in \mathbb{R}^2$ and $W > 0$, with density

$$\frac{e^{-|\nu|^2/c^2}}{\pi c^2} \frac{2\omega e^{-\omega^2/c^2}}{c^2}, \quad \nu \in \mathbb{R}^2, \quad \omega > 0. \quad (9.1)$$

The parameter c equals $\sqrt{2kT/m}$, with T = absolute temperature, m = mass per gas molecule, and k = Boltzmann constant; dimensionally, c is a speed. The reflection law at the upper wall, $z = 1$, is analogous, with the sign of W reversed.

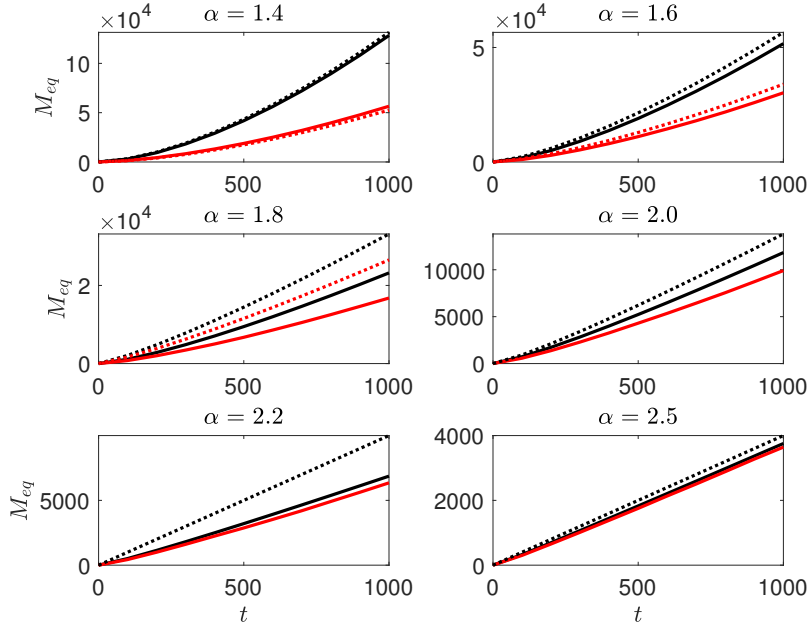


Fig. 8.1: Red: M_{tr} (solid, computed by Monte Carlo simulation) and leading asymptotic approximation for M_{tr} (dotted). Black: M_{eq} (solid, computed analytically) and leading asymptotic approximation for M_{eq} (dotted). For $\alpha \geq 2$, the leading asymptotic approximations for M_{tr} and M_{eq} are identical, and are shown as black dotted curves.

The time τ between a collision with a wall and the next collision with the opposite wall equals $1/|W|$. The distribution function of τ is

$$F(t) = P(\tau \leq t) = P\left(|W| \geq \frac{1}{t}\right) = \int_{1/t}^{\infty} \frac{2\omega e^{-\omega^2/c^2}}{c^2} d\omega = e^{-1/(ct)^2}.$$

Note also that

$$F(t) = 1 - \frac{1}{(ct)^2} + \frac{1}{2(ct)^4} - \dots \quad \text{as } t \rightarrow \infty. \quad (9.2)$$

The mean of τ is

$$\bar{\tau} = \int_0^{\infty} \left(1 - e^{-1/(ct)^2}\right) dt = \frac{\sqrt{\pi}}{c}. \quad (9.3)$$

The two components of the horizontal velocity V are Gaussians with mean zero and variance $c^2/2$, independent of each other and of W . Therefore

$$v^2 = E(|V|^2) = E(V_1^2 + V_2^2) = c^2.$$

From Proposition 3.3, M_{eq} can be expressed in terms of the error function erf and the exponential integral Ei . We omit the unwieldy formula, which however makes it

easy to find asymptotic expansions of M_{eq} to arbitrary accuracy. For instance, we find

$$M_{eq}(t) = \frac{2ct \log(ct)}{\sqrt{\pi}} + \frac{1-\gamma}{\sqrt{\pi}} ct + \frac{2}{3} + O\left(\frac{1}{t}\right) \quad \text{as } t \rightarrow \infty, \quad (9.4)$$

where $\gamma \approx 0.577$ is the Euler-Mascheroni constant. Using eq. (8.2) and Lemma 8.4, we also conclude

$$M_{tr}(t) = \frac{2ct \log(ct)}{\sqrt{\pi}} - \frac{1+\gamma}{\sqrt{\pi}} ct + O\left(t^{1/2}(\log t)^{3/2}\right) \quad (9.5)$$

for the transitional mean square displacement.

It is interesting to compare (9.4) and (9.5) with the main result of [5]. The notation in [5] differs from that used here in several ways. In particular, in the limit studied in [5], the channel width tends to zero while time tends to infinity. However, it is not difficult to show that the result of [5], translated into the notation used here, predicts that at time t , the distribution of the location of a particle starting at the origin at time 0 will be approximately bivariate Gaussian with variance

$$\frac{ct \log(ct)}{\sqrt{\pi}}.$$

Comparing with (9.4) we see the “doubling effect” previously observed by others [2, 3, 30] in which the variance of the long-time Gaussian approximation is half the leading-order MSD approximation.

10. Summary. There is considerable interest in the MSD in Lévy walks due to the importance of this quantity in a wide variety of application areas. The leading-order behavior of MSDs for Lévy walks with power law distributions of the flight segment duration is asymptotically determined by the exponent of the power law, up to a constant of proportionality. Given a mean duration, the constant of proportionality is determined as well. However, the quality of the asymptotic approximation depends delicately on the exact form of the distribution. The dependence is especially sensitive for power laws with exponents near 2. At $\alpha = 2$, the leading-order term of the MSD at time t is proportional to $t \log t$, but the next-order term is usually proportional to t , with a constant of proportionality which depends on the entire distribution. For α near 2, the sub-leading-order terms can also be close to the leading-order terms for values of t of physical interest.

We have derived exact, closed-form expressions, valid for all time, for the MSDs for particular choices of the power laws and for a power law perturbed by a logarithmic factor. These examples illustrate the dependence of the accuracy of the asymptotics on the entire distribution. We have also established robustness of the MSD asymptotics in the sense that power law bounds on the distribution functions imply power law bounds on the equilibrium MSDs. Finally, we have proved that for power laws with α between 1 and 2, the equilibrium and transitional MSDs are asymptotically proportional, with constant of proportionality $\alpha - 1$.

Acknowledgment. The second author thanks the Courant Institute for hosting him as a Visiting Scholar.

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