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Classical localization for the drift–diffusion equation on a Cayley tree

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Abstract. We show that classical localization occurs for the drift–diffusion equation on an ordered Cayley tree when the drift velocity v on each branch of the tree exceeds a critical value $v_c = DL^{-1}\ln(z-1)$, where z is the coordination number, D is the diffusion constant and L is the segment length. For $v < v_c$ the asymptotic decay of the delocalized state exhibits conventional diffusive behaviour, whereas at the critical point $v = v_c$ there is anomalous behaviour in the form of a critical slowing-down. A necessary condition for localization in the presence of randomly distributed drift velocities is also derived.

Physical processes defined on Cayley trees or Bethe lattices exhibit many non-trivial features whilst remaining analytically tractable, the absence of loops being a key factor. The study of biased random walks on a Bethe lattice, both in discrete time [1] and continuous time [2, 3], reveals interesting and indeed anomalous diffusive behaviour. It is interesting, therefore, to consider how such behaviour manifests itself in an analogous continuum system, namely the drift–diffusion equation on a Cayley tree.

Consider an unbounded Cayley tree Γ with coordination number z and segment length L. Choose the origin to be a particular branching node $\alpha_0 \in \Gamma$ (see figure 1). For each segment k of the tree, denote the node closer to α_0 by $\alpha'(k)$ and the one further away by $\alpha(k)$. Introduce a local coordinate x on each segment such that $x(\alpha(k)) = L$ and $x(\alpha'(k)) = 0$. For each branching node α label the set of segments radiating from it by $\mathcal{I}_\alpha$. Let $\tilde{\mathcal{I}}_\alpha$ denote the set of line segments $k \in \mathcal{I}_\alpha$ that radiate from α in a positive x-direction; the number of elements of $\tilde{\mathcal{I}}_\alpha$ is thus $z-1$. Using these various definitions we can introduce the idea of a generation. The first generation consists of the z segments $\Sigma_1 = \{k \in \mathcal{I}_{\alpha_0}\}$, the second generation consists of the $z(z-1)$ segments $\Sigma_2 = \{l, l \in \tilde{\mathcal{I}}_{\alpha(k)}, k \in \Sigma_1\}$, etc.

Suppose that $c_i(x, t)$, which denotes the concentration at position x and time t on the ith segment of the tree, evolves according to the drift–diffusion equation

$$\frac{\partial c_i}{\partial t} = D\frac{\partial^2 c_i}{\partial x^2} + v\frac{\partial c_i}{\partial x} \qquad t > 0 \qquad 0 < x < L. \tag{1}$$

Here D is the diffusion constant and v is the drift velocity, which is taken to be inwards with respect to the origin α_0 (see figure 1). Equation (1) is supplemented by the boundary conditions expressing continuity of the concentration at the node,

$$c_i(x(\alpha), t) = c_k(x(\alpha), t) \qquad \text{for all } i, k \in \mathcal{I}_\alpha \qquad t > 0 \tag{2}$$

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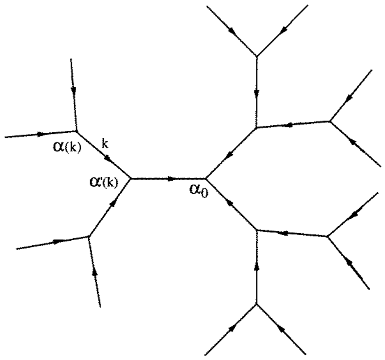

Figure 1. Cayley tree with all drift velocities in the direction of branching node α_0.

and conservation of current through the node,

$$\sum_{i\in\mathcal{I}_\alpha} \eta_i J_i(x(\alpha), t) = 0 \qquad J_i(x, t) = -D\frac{\partial c_i}{\partial x} - vc_i \qquad t > 0 \tag{3}$$

where $\eta_i = +1(\eta_i = -1)$ if $x(\alpha) = 0(x(\alpha) = L)$. For later convenience, we shall denote the concentration at a node α by $\Phi_\alpha(t)$.

In this paper we are interested in the following classical localization problem: given initial data consisting of a unit impulse located at α_0 at time $t = 0$, what is the asymptotic behaviour of the on-site amplitude $\Phi_{\alpha_0}(t)$? In the absence of drift, it is clear that the on-site amplitude $\Phi_{\alpha_0}(t)$ decays to zero as $t \to \infty$ due to the effects of diffusion. In other words, the steady state is delocalized. However, as one switches on a positive inwards drift velocity v one expects the effects of diffusion away from α_0 to be counteracted by the drift such that beyond some critical velocity v_c there is a non-zero steady state, $\lim_{t\to\infty} \Phi_{\alpha_0}(t) \neq 0$. The system is then said to be localized. The critical velocity should increase with the coordination number z since the delocalizing effect of diffusion grows with z. An analogous problem was previously investigated within the context of biased random walks on a Bethe lattice, both in discrete time [1] and continuous time [2, 3].

Before studying the full time-dependent solution to equations (1)–(3), it is useful to consider the steady-state case. The steady-state concentration $c_i(x)$ on segment i satisfies

$$-J_i \equiv D\frac{\partial c_i}{\partial x} + vc_i = 0. \tag{4}$$

By symmetry, all segments belonging to the same generation will have an identical solution: for the $z(z-1)^{p-1}$ segments of the pth generation, $p \geqslant 1$, the solution is $A_p \mathrm{e}^{-vx/D}$. The coefficients A_p are related by imposing continuity at the branching nodes, $A_{p+1} = A_p \mathrm{e}^{-vL/D}$. Hence

$$c_i(x) = A_1 \mathrm{e}^{-v(pL-L+x)/D} \qquad i \in \Sigma_p. \tag{5}$$

Conservation of particle number implies that

$$\sum_i \int_0^L c_i(x)\,\mathrm{d}x = 1. \tag{6}$$

Substituting equation (5) into equation (6) then gives

$$1 = \frac{A_1 z D}{v} \sum_{p=0}^{\infty} (z-1)^p \mathrm{e}^{-pvL/D}[1 - \mathrm{e}^{-vL/D}]. \tag{7}$$

Equation (7) leads to the following localization criterion: a non-zero steady state $\lim_{t\to\infty}\Phi_{\alpha_0}(t) = A_1$ occurs if the infinite series on the right-hand side of equation (7) is convergent. This yields the critical velocity

$$v_c = \frac{D}{L}\ln(z-1) \tag{8}$$

and for $v > v_c$,

$$\lim_{t\to\infty}\Phi_{\alpha_0}(t) = \frac{v[1-(z-1)e^{-vL/D}]}{zD[1-e^{-vL/D}]}. \tag{9}$$

In order to determine the rate of decay of the delocalized state at or below criticality, it is necessary to solve the full equations (1)–(3). One approach would be to Laplace-transform the drift–diffusion equation on each line segment i and then to use transfer matrices. We shall follow a different approach here, which is similar in spirit to one developed within the context of the linearized Landau–Ginzburg equation describing networks of superconducting wires [4]. (See also the analysis of Schrödinger's equation on quantum wire networks [5]; note that Ringwood [6] used transfer matrices to solve the Schrödinger equation on a Cayley tree but, unfortunately, his final expression for the Green function was incorrect.) The basic idea is to solve the drift–diffusion equation on each line segment in terms of the as yet unknown time-dependent functions $\Phi_\alpha(t)$ specifying the concentration at the branching nodes α; the functions $\Phi_\alpha(t)$ are then determined self-consistently by imposing current conservation at each branching node (continuity is automatically satisfied). First, introduce the initial data $c_i(x,0) = \delta(x-a)\delta_{i,j}$ where j is a particular segment attached to node α_0. (The choice of $j \in \mathcal{I}_\alpha$ is unimportant, since we shall eventually take the limit $a \to 0$.) An application of Green's theorem [7] then gives

$$c_i(x,t) = G(x,t|a,0)\delta_{i,j} + D\int_0^t \left[\left.\frac{\partial}{\partial x'}\right|_{x'=0} G(x,t|x',t')\Phi_{\alpha'(i)}(t') - \left.\frac{\partial}{\partial x'}\right|_{x'=L} G(x,t|x',t')\Phi_{\alpha(i)}(t')\right] dt' \tag{10}$$

where $G(x,t|x',0)$ is the fundamental solution on a finite segment of length L with homogeneous open boundary conditions at both ends. The latter can be calculated explicitly [7]:

$$G(x,t|x',t') = \frac{\exp\left(\frac{-(x-x')v}{2D} - \frac{v^2(t-t')}{4D}\right)}{\sqrt{4\pi D(t-t')}} \times \sum_{k=-\infty}^{\infty}[e^{-(x-x'+2kL)^2/4D(t-t')} - e^{-(x+x'+2kL)^2/4D(t-t')}]. \tag{11}$$

Substitution of equation (10) into the current conservation condition (3) leads to a set of coupled linear integral equations for the functions $\Phi_\alpha(t)$. Performing a Laplace transform of equations (3), (10) and (11) with

$$\tilde{G}(x,x';s) = \frac{\exp\left(\frac{-(x-x')v}{2D}\right)}{2D\hat{s}}\,\frac{e^{-(x-x')\hat{s}} + e^{-(2L-|x-x'|)\hat{s}} - e^{-(x+x')\hat{s}} - e^{-(2L-x-x')\hat{s}}}{1-e^{-2L\hat{s}}} \tag{12}$$

where $\hat{s} = \sqrt{(s+\epsilon)/D}$ and $\epsilon = \frac{v^2}{4D}$, results in a corresponding set of coupled linear equations for the Laplace-transformed concentrations $\tilde{\Phi}_\alpha(s)$. In the limit $a \to 0$, these take the relatively simple form

$$1 - H_0(s)\tilde{\Phi}_{\alpha_0}(s) + \sum_{k\in\mathcal{I}_{\alpha_0}}\bar{g}(s)\tilde{\Phi}_{\alpha(k)}(s) = 0 \tag{13}$$

and for $k \in \Sigma_p$

$$-H(s)\tilde{\Phi}_{\alpha(k)}(s) + g(s)\tilde{\Phi}_{\alpha'(k)}(s) = -\sum_{l\in\bar{\mathcal{I}}_{\alpha(k)}} \bar{g}(s)\tilde{\Phi}_{\alpha(l)}(s). \tag{14}$$

Here

$$\begin{aligned} g(s) &= \mathrm{e}^{-Lv/2D}\frac{\sqrt{(s+\epsilon)D}}{\sinh(L\sqrt{(s+\epsilon)/D})} \qquad \bar{g}(s) = \mathrm{e}^{Lv/2D}\frac{\sqrt{(s+\epsilon)D}}{\sinh(L\sqrt{(s+\epsilon)/D})} \\ H(s) &= s\sqrt{(s+\epsilon)D}\coth\left(L\sqrt{(s+\epsilon)/D}\right) - \frac{(z-2)v}{2} \qquad H_0(s) = H(s) - v. \end{aligned} \tag{15}$$

It is clear from equations (13) and (14) that the solution at every branching node $\alpha(k)$ associated with the same generation p is identical. Thus we set $\tilde{\Phi}_{\alpha(k)} = \tilde{\Phi}_p$ for all $k \in \Sigma_p$, $p \geqslant 1$. Equations (13) and (14) can then be written in the form

$$1 - H_0(s)\tilde{\Phi}_{\alpha_0}(s) + z\bar{g}(s)\tilde{\Phi}_1(s) = 0 \tag{16}$$

$$-H(s)\tilde{\Phi}_p(s) + g(s)\tilde{\Phi}_{p-1}(s) + (z-1)\bar{g}(s)\tilde{\Phi}_{p+1}(s) = 0 \qquad p \geqslant 1 \tag{17}$$

where $\tilde{\Phi}_0(s) \equiv \tilde{\Phi}_{\alpha_0}(s)$. The solution of the difference equation (17) is

$$\tilde{\Phi}_p(s) = \left[\frac{g(s)}{\lambda(s)}\right]^p \tilde{\Phi}_{\alpha_0}(s) \tag{18}$$

where

$$\lambda(s) = \tfrac{1}{2}\left[H(s) + \sqrt{H(s)^2 - 4(z-1)g(s)\bar{g}(s)}\right]. \tag{19}$$

Substitution of equation (18) into (16) finally yields the result

$$\tilde{\Phi}_{\alpha_0}(s) = \left[H_0(s) - \frac{zg(s)\bar{g}(s)}{\lambda(s)}\right]^{-1}. \tag{20}$$

The expression for the Laplace transform $\tilde{\Phi}_{\alpha_0}(s)$, equation (20), can be used to determine both the critical velocity v_c and the asymptotic behaviour of the on-site amplitude $\Phi_{\alpha_0}(t)$ at the critical point. First, note that $\lim_{t\to\infty}\Phi_{\alpha_0}(t) = \lim_{s\to 0} s\tilde{\Phi}_{\alpha_0}(s)$. Thus localization will occur if and only if $\tilde{\Phi}_{\alpha_0}(s) \sim s^{-1}$ for small s. A necessary but not sufficient indicator of localization, which will be used later for the disordered Cayley tree, is that $\lim_{s\to 0}\tilde{\Phi}(s) = \infty$. It is useful to rewrite equation (20) in the form

$$\tilde{\Phi}_{\alpha_0}(s) = \frac{2\lambda(s)}{H_0(s)}[\lambda_0(s) + \lambda_1(s)]^{-1} \tag{21}$$

with

$$\lambda_0(s) = H(s) - \frac{zg(s)\bar{g}(s)}{H_0(s)} \qquad \lambda_1(s) = \sqrt{H(s)^2 - 4(z-1)g(s)\bar{g}(s)}. \tag{22}$$

One finds that

$$\lambda_0(0) = \frac{\sqrt{\epsilon D}}{\sinh L\sqrt{\epsilon/D}}[\mathrm{e}^{-\sqrt{\epsilon/D}L}(z-1) - \mathrm{e}^{\sqrt{\epsilon/D}L}] \qquad \lambda_1(0) = |\lambda_0(0)|. \tag{23}$$

Equation (23) implies that if $\lambda_0(0) > 0$ then $\tilde{\Phi}_{\alpha_0}(0) \neq 0$ and the steady state is delocalized. On the other hand, if $\lambda_0(0) < 0$ then $\lambda_0(s) + \lambda_1(s) \sim s$ for small s and we do have localization. Thus the critical velocity is determined from the condition $\lambda_0(0) = 0$ and we recover equation (8). At the critical velocity $v = v_\mathrm{c}$, $\lambda_1(s) \sim \sqrt{s}$ for small s and this will dominate the behaviour of $\tilde{\Phi}_{\alpha_0}(s)$, that is, $\tilde{\Phi}_{\alpha_0}(s) \sim 1/\sqrt{s}$. Therefore, at the critical velocity $v = v_c$ we can apply a Tauberian theorem [8] to deduce that

$$\Phi_{\alpha_0}(t) \sim \frac{1}{\sqrt{\pi t D}} \frac{\sqrt{z-1}}{z} \qquad t \to \infty. \tag{24}$$

Equation (24) shows that the solution exhibits a slower rate of decay than expected for conventional drift–diffusion. In other words, as found for biased random walks [3], there is critical slowing down. It is also interesting to note that the critical behaviour is independent of the segment length L.

In order to determine the asymptotic behaviour of the on-site amplitude $\Phi_{\alpha_0}(t)$ below the critical point ($v < v_c$), we need to invert equation (20). In the simple case $z = 2$, the Cayley tree reduces to two semi-lines joined at the origin $x = 0$ with drift velocities moving towards the origin. Then equation (20) becomes

$$\tilde{\Phi}_{\alpha_0}(s) = \frac{1}{2\sqrt{(s+\epsilon)D} - v} \tag{25}$$

which is easily inverted to yield

$$\Phi_{\alpha_0}(t) = \frac{1}{2}\left[\frac{e^{-v^2 t/4D}}{\sqrt{\pi t D}} + \frac{v}{2D}\,\mathrm{erfc}\left(\frac{-v}{2}\sqrt{\frac{t}{D}}\right)\right] \tag{26}$$

where $\mathrm{erfc}(x) = 2\pi^{-1/2}\int_x^\infty e^{-y^2}\,dy$. It follows from equation (26) that $\lim_{t\to\infty}\Phi_{\alpha_0}(t) = v/2D$ for $v > 0$ and $\lim_{t\to\infty}\Phi_{\alpha_0}(t) = 0$ for $v < 0$, which agrees with equations (8) and (9) when $z = 2$. The asymptotic behaviour of the delocalized state is

$$\begin{aligned} \Phi_{\alpha_0}(t) &\sim \frac{1}{2\sqrt{\pi t D}} \qquad v = 0 \\ \Phi_{\alpha_0}(t) &\sim \frac{2D^2}{\sqrt{\pi}v^2}\frac{e^{-v^2 t/4D}}{(Dt)^{3/2}} \qquad v < 0. \end{aligned} \tag{27}$$

Inverting equation (20) when $z > 2$ requires performing a Bromwich contour integral. It can be shown that for $v < v_c$ the function $\tilde{\Phi}_{\alpha_0}(s)$ has an infinite set of branch points along the negative real axis of the complex s-plane. These are given by $s = X^2 - \epsilon$ where X is a root of the transcendental equation

$$\cosh X - \frac{vL}{2D}\frac{z-2}{z}\frac{\sinh X}{X} = \pm\frac{2\sqrt{z-1}}{z}. \tag{28}$$

Equation (28) has an infinite number of imaginary roots and at most one real root. The asymptotic behaviour of $\Phi_{\alpha_0}(t)$ below criticality arises from the contribution to the Bromwich integral in the region of the branch point closest to $s = 0$. (As $v \to v_c$ this branch point approaches $s = 0$ resulting in the $1/\sqrt{s}$ behaviour at criticality.) We find that for large t and for $v < v_c$ such that a real root X_1 of equation (28) exists,

$$\Phi_{\alpha_0}(t) \sim \left(\frac{K_X X_1\sqrt{z-1}}{2z\pi D t^3}\right)^{1/2} \frac{\exp\left(-\left[\frac{v^2}{4D} - \frac{DX_1^2}{L^2}\right]t\right)}{\left[\frac{v^2}{4D} - \frac{DX_1^2}{L^2}\right]\sinh X_1} \tag{29}$$

where

$$K_X = \sinh X_1 - \frac{vL}{2D}\frac{z-2}{z}\left(\cosh X_1 - \frac{\sinh X_1}{X_1}\right). \tag{30}$$

Note that as v decreases, $X_1 \to 0$ and then becomes imaginary. Thus for v sufficiently below the critical point, there is no real root of equation (28) and the asymptotic behaviour is dominated by the smallest magnitude imaginary root $X_1 = \mathrm{i}Y_1$. Then

$$\Phi_{\alpha_0}(t) \sim \left(\frac{K_Y Y_1\sqrt{z-1}}{2z\pi D t^3}\right)^{1/2} \frac{\exp\left(-\left[\frac{v^2}{4D} + \frac{DY_1^2}{L^2}\right]t\right)}{\left[\frac{v^2}{4D} + \frac{DY_1^2}{L^2}\right]\sin Y_1} \tag{31}$$

with

$$K_Y = \sin Y_1 - \frac{vL}{2D}\frac{z-2}{z}\left(\cos Y_1 - \frac{\sin Y_1}{Y_1}\right). \tag{32}$$

Note that if $z = 2$ then $K_X = \sinh X_1$ and $X_1 \to 0$ such that $(K_X X_1)^{1/2}/\sinh X_1 \to 1$, and we recover equation (27).

So far we have assumed that the drift velocity is identical on all segments of the tree. Now suppose that the drift velocity v_i on branch i is independently chosen at random from a given probability density $\rho(v)$. In the one-dimensional case, $z = 2$, this problem is completely solvable analytically (see Bouchaud and Georges [9] and references therein). Aslangul *et al* [10] have extended the one-dimensional analysis to the case of a biased random walk on a directed Bethe lattice where particles can only move in the direction of increasing generation number. Unfortunately, the latter does not yield a drift–diffusion equation in the continuum limit and the analysis breaks down. Nevertheless, it is possible to make some progress by considering a slightly easier problem; assume that for each generation p, $v_i = v_p$ for all $i \in \Sigma_p$ with v_p independently chosen at random from $\rho(v)$. In other words, there is intergenerational but not intragenerational randomness.

In order to investigate the onset of localization, we shall calculate the average Laplace transform $\langle\tilde{\Phi}_p(0)\rangle$. Following the analysis of one-dimensional continuous-time random walks [9], we define

$$U^{-1} = \lim_{p\to\infty}(z-1)^p\langle\tilde{\Phi}_p(0)\rangle \tag{33}$$

with U interpreted as an asymptotic particle velocity; a necessary but not sufficient criterion for localization is that U vanishes. To determine U, we first Laplace-transform equation (1) assuming initial data in the form of an impulse at α_0:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(D\frac{\mathrm{d}\tilde{c}_p(x,s)}{\mathrm{d}x} + v_p\tilde{c}_p(x,s)\right) = -\delta_{p,1}\delta(x) + s\tilde{c}_p(x,s) \tag{34}$$

where, by symmetry, $c_i = c_p$ for all $i \in \Sigma_p$. Equation (34) is supplemented by the current conservation condition

$$D\frac{\mathrm{d}\tilde{c}_p(L,s)}{\mathrm{d}x} + v_p\tilde{c}_p(L,s) = +(z-1)\left[D\frac{\mathrm{d}\tilde{c}_{p+1}(0,s)}{\mathrm{d}x} + v_{p+1}\tilde{c}_{p+1}(0,s)\right]. \tag{35}$$

Setting $s = 0$ and then integrating equation (34) yields, when current conservation is incorporated,

$$D\frac{\mathrm{d}\tilde{c}_p(x,0)}{\mathrm{d}x} + v_p\tilde{c}_p(x,0) = -\frac{1}{(z-1)^p}. \tag{36}$$

This has the solution

$$\tilde{c}_p(x,0) = \tilde{\Phi}_p(0)\mathrm{e}^{-v_p x/D} - \frac{1}{v_p(z-1)^p}[1 - \mathrm{e}^{-v_p x/D}]. \tag{37}$$

Continuity at the branching nodes gives the first-order difference equation

$$B_p = \frac{e^{v_p L/D} - 1}{v_p} + \frac{e^{v_p L/D}}{z-1} B_{p+1} \qquad B_p = (z-1)^p \tilde{\Phi}_p(0). \tag{38}$$

Iterating equation (38),

$$B_p = \frac{e^{v_p L/D} - 1}{v_p} + \sum_{j=1}^{N-1} \frac{e^{v_{p+j} L/D} - 1}{v_{p+j}} \prod_{k=0}^{j-1} \frac{e^{v_{p+k} L/D}}{z-1} + \prod_{k=0}^{N-1} \frac{e^{v_{p+k} L/D}}{z-1} B_{p+N}. \tag{39}$$

Averaging equation (39) with respect to $\rho(v)$,

$$\langle B_p \rangle = \left\langle \frac{e^{vL/D} - 1}{v} \right\rangle \left\{ 1 + \sum_{k=1}^{N-1} \left\langle \frac{e^{vL/D}}{z-1} \right\rangle^k \right\} + \left\langle \frac{e^{vL/D}}{z-1} \right\rangle^N \langle B_{p+N} \rangle. \tag{40}$$

Finally, taking the limit $N \to \infty$ we have

$$\begin{aligned} \langle B_p \rangle &= \infty \qquad \text{if } \left\langle \frac{e^{vL/D}}{z-1} \right\rangle > 1 \\ \langle B_p \rangle &= \left\langle \frac{e^{vL/D} - 1}{v} \right\rangle \left\langle 1 - \frac{e^{vL/D}}{z-1} \right\rangle^{-1} \qquad \text{if } \left\langle \frac{e^{vL/D}}{z-1} \right\rangle < 1. \end{aligned} \tag{41}$$

(Note that intergenerational disorder in the coordination number is also handled by the above analysis.)

Assuming that the weak criterion for localization ($U = 0$) is valid, equation (41) implies that classical localization for the drift–diffusion equation on a disordered Cayley tree with intergenerational randomness can only occur when $\langle e^{vL/D} \rangle > (z-1)$. As an example, consider the Bernoulli distribution $\rho(v) = p\delta(v - \bar{v}) + (1-p)\delta(v + \bar{v})$. A simple calculation shows that U vanishes if and only if $\bar{v} > v_c(p)$ where

$$v_c(p) = \frac{D}{L} \ln \left\{ \frac{z - 1 + \sqrt{(z-1)^2 - 4(1-p)p}}{2p} \right\}. \tag{42}$$

Finally, we point out that certain care must be taken over the interpretation of equation (41), since we have not established that the asymptotic particle velocity U is self-averaging. However, by analogy with results from continuous-time random walks [9, 10], we expect that self-averaging does hold. In order to prove this, we would need to determine the behaviour of the solution $\langle \tilde{\Phi}_p(s) \rangle$ for non-zero s. This would require extending some of the techniques of one-dimensional random walks [9]. Alternatively, one might be able to exploit certain formal similarities between the recursive equations (13) and (14) and those derived for Ricatti variables associated with the Anderson model on a Cayley tree [11]. This will be considered in more detail elsewhere, together with other issues such as the effects of intragenerational disorder.

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