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On the Wang–Uhlenbeck Problem in Discrete Velocity Space

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The arguably simplest model for dynamics in phase space is the one where the velocity can jump between only two discrete values, $\pm v$, with rate constant k. For this model, which is the continuous-space version of a persistent random walk, analytic expressions are found for the first passage time distributions to the origin. Since the evolution equation of this model can be regarded as the two-state finite-difference approximation in velocity space of the Kramers–Klein equation, this work constitutes a solution of the simplest version of the Wang–Uhlenbeck problem. Formal solution (in Laplace space) of generalizations where the velocity can assume an arbitrary number of discrete states that mimic the Maxwell distribution is also provided.

KEY WORDS: First passage times; persistent random walk; Kramers equation.

1. INTRODUCTION

In their classical review, Wang and Uhlenbeck(1) posed the problem of finding the distribution of the first-passage times to the origin of a particle freely diffusing in phase space. The dynamics of such a particle can be described by the stochastic Langevin equation or equivalently by the Kramers–Klein equation(2) equation for the joint position and velocity distribution function, $P(x, v, t)$. In coordinate space, where the dynamics is described by the ordinary diffusion (parabolic) equation, this problem is simply solved. In phase space, this problem is considerably more difficult

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not only because of the two dimensionality of the evolution (elliptic) equation but also due to the nature of the absorbing boundary condition at the origin which involves only particles moving with the appropriate velocity [i.e., $P(0, v, t) = 0$ for $v > 0$ when the initial position is $x_0 > 0$]. It took over forty years before Marshall and Watson,[3] using sophisticated techniques, were able to derive an expression for the Laplace transform of the first-passage-time distribution. Their expression, which involves coefficients that could only be obtained by a limiting procedure, is so complicated that it is unlikely that it can be inverted into the time domain.

In this paper we consider the Wang–Uhlenbeck problem in the discrete velocity space. When the velocity can assume only two values, all the essential features of the original problem are retained, yet the first-passage-time distribution can be analytically found in the time domain. Consider a particle moving in one dimension whose velocity stochastically fluctuates between just two values, $\pm v$. The interconversion between the "+" and "−" velocity states is described by the kinetic scheme $-v \underset{k}{\overset{k}{\rightleftharpoons}} v$, where k is the transition rate constant [i.e., a Poisson process]. The evolution equation [see below] of this problem is two dimensional [continuous in space but discrete in velocity] and can be regarded as the simplest finite difference approximation [for the velocity] of the Kramers–Klein equation.[2] It also describes the continuous space analogue of a persistent random walk introduced by Taylor[4] in an attempt to treat turbulent diffusion. As shown by Goldstein,[5] it is equivalent to the telegrapher's equation which governs the flow of electricity in cables. Masoliver *et al.*[6] studied the solutions of the telegrapher's equation subject to a variety of boundary conditions [including absorbing]. They focused primarily on the velocity averaged conditional probability density for finding the system at a given position and did not explicitly consider the dependence of the survival probability on the initial velocity.

For the above model, the probability densities, $P_\pm(x, t)$ that the particle is at x at time t with velocity $\pm v$ satisfy:

$$\frac{\partial}{\partial t}\begin{pmatrix} P_+ \\ P_- \end{pmatrix} = \mathbf{L}\begin{pmatrix} P_+ \\ P_- \end{pmatrix} \tag{1a}$$

$$\mathbf{L} = \begin{pmatrix} -v\dfrac{\partial}{\partial x} - k & k \\ k & v\dfrac{\partial}{\partial x} - k \end{pmatrix} \tag{1b}$$

The average velocity is zero while $\langle v^2 \rangle_{\text{eq}} = v^2$. The velocity autocorrelation function, $\langle v(t)\, v(0) \rangle_{\text{eq}} / \langle v^2 \rangle_{\text{eq}} = e^{-2kt}$, is a single exponential just like for the Kramers-Klein equation. However, $\langle v^4 \rangle_{\text{eq}} = (\langle v^2 \rangle_{\text{eq}})^2$ rather than $\langle v^4 \rangle_{\text{eq}} = 3(\langle v^2 \rangle_{\text{eq}})^2$, which holds for a Maxwellian distribution of velocities.

We treat $x=0$ as an absorbing point. Let $S_\pm(t \mid x)$ be the survival probability of a particle initially at x $[x>0]$ with velocity $\pm v$. The distribution of first passage times to $x=0$ for the particle initially at x $[x>0]$ with velocity $\pm v$, denoted by $F_\pm(t \mid x)$, are related to the survival probabilities via $F_\pm(t \mid x) = -\partial S_\pm(t \mid x)/\partial t$. The survival probabilities satisfy the adjoint equation:

$$\frac{\partial}{\partial t}\begin{pmatrix} S_+ \\ S_- \end{pmatrix} = \mathbf{L}^\dagger \begin{pmatrix} S_+ \\ S_- \end{pmatrix} \tag{2a}$$

$$\mathbf{L}^\dagger = \begin{pmatrix} v\dfrac{\partial}{\partial x} - k & k \\ k & -v\dfrac{\partial}{\partial x} - k \end{pmatrix} \tag{2b}$$

since $(\partial/\partial x)^\dagger = -\partial/\partial x$. The initial conditions are $S_\pm(t=0 \mid x) = 1$ and the boundary condition is:

$$S_-(t \mid x=0) = 0 \tag{3}$$

since a particle initially at $x>0$ is absorbed by the boundary at $x=0$ only when it is moving with a negative velocity. This is the adjoint of the Wang and Uhlenbeck boundary condition for the probability density. The survival probability of a particle initially at $x=0$ but moving with velocity $+v$ [i.e., $S_+(t \mid 0)$] is non zero and is to be determined. At first sight, the boundary condition in Eq. (3) does not appear to be sufficient to find a unique solution to the coupled pair of first order differential equation (2a, 2b). As we show below, a unique solution can be found by imposing the requirement that the survival probabilities must be finite as $x \to \infty$, i.e., the generalized albedo problem.[3]

Laplace transforming Eq. (2a) $[\mathscr{L}[g] = \hat{g}(\sigma) = \int_0^\infty e^{-\sigma t} g(t)\, dt]$, we find:

$$\frac{\partial}{\partial x}\begin{pmatrix} \hat{S}_+ \\ \hat{S}_- \end{pmatrix} = \mathbf{M}\begin{pmatrix} \hat{S}_+ \\ \hat{S}_- \end{pmatrix} + \frac{1}{v}\begin{pmatrix} -1 \\ 1 \end{pmatrix} \tag{4}$$

where we have used the initial conditions $S_\pm(0 \mid x) = 1$ and defined $\mathbf{M}$ by:

$$\mathbf{M} = \frac{1}{v}\begin{pmatrix} \sigma + k & -k \\ k & -\sigma - k \end{pmatrix} \tag{5}$$

The σ-dependent eigenvalues λ_1 and λ_2 and corresponding eigenvectors $\mathbf{u}_1$ and $\mathbf{u}_2$ of $\mathbf{M}$ are:

$$\left.\begin{matrix}\lambda_1\\ \lambda_2\end{matrix}\right\} = \pm\lambda; \qquad \lambda = \frac{\sqrt{\sigma(\sigma+2k)}}{v},$$

and

$$\mathbf{u}_{1,2} = \begin{pmatrix} 1 \\ c_{1,2} \end{pmatrix}; \qquad c_{1,2} = \frac{k}{\sigma + k \pm \lambda v} \tag{6}$$

The general solution of Eq. (4) is therefore:

$$\begin{pmatrix} \hat{S}_+(\sigma \mid x) \\ \hat{S}_-(\sigma \mid x) \end{pmatrix} = \frac{1}{\sigma}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + A e^{\lambda x}\begin{pmatrix} 1 \\ c_1 \end{pmatrix} + B e^{-\lambda x}\begin{pmatrix} 1 \\ c_2 \end{pmatrix} \tag{7}$$

where A and B are unknown constants. For the survival probabilities to be bounded as $x \to \infty$ we must set $A = 0$. The remaining constant B is obtained using the boundary condition in Eq. (3) and we have:

$$\hat{S}_+(\sigma \mid x) = \frac{1}{\sigma}\left[1 - \left(\frac{\sigma + k - v\lambda}{k}\right) e^{-\lambda x}\right] \tag{8a}$$

$$\hat{S}_-(\sigma \mid x) = \frac{1}{\sigma}\left[1 - e^{-\lambda x}\right] \tag{8b}$$

Since $F_\pm(t \mid x) = -\partial S_\pm(t \mid x)/\partial t$, the Laplace transforms of the first passage time distribution functions are:

$$\hat{F}_+(\sigma \mid x) = \left(\frac{\sigma + k - v\lambda}{k}\right) e^{-\lambda x} \tag{9a}$$

$$\hat{F}_-(\sigma \mid x) = e^{-\lambda x} \tag{9b}$$

The key relation we need to invert these Laplace transform is:[7]

$$\mathscr{L}^{-1}\left[\frac{e^{-a\sqrt{(\sigma+b_1)(\sigma+b_2)}}}{\sqrt{(\sigma+b_1)(\sigma+b_2)}}\right] = \mathrm{H}(t-a)\, e^{-(b_1+b_2)t/2} \mathrm{I}_0\left[\frac{b_1 - b_2}{2}\sqrt{t^2 - a^2}\right] \tag{10}$$

where $\mathscr{L}^{-1}[\cdots]$ denotes the inverse Laplace transform, $\mathrm{I}_0[\cdots]$ is the modified Bessel function of order zero and $\mathrm{H}(\cdots)$ is the Heaviside step function defined as $\mathrm{H}(x) = 0$ for $x < 0$ and $\mathrm{H}(x) = 1$ for $x > 0$. Differentiating this with respect to a and using the convolution relation, we finally find:

$$F_+(t\mid x) = \mathrm{H}\left(t - \frac{x}{v}\right)\frac{\mathrm{e}^{-kt}}{(t+x/v)} \times \left\{\frac{xk}{v}\,\mathrm{I}_0\left[k\sqrt{t^2-\frac{x^2}{v^2}}\right] + \left(\frac{t-x/v}{t+x/v}\right)^{1/2}\mathrm{I}_1\left[k\sqrt{t^2-\frac{x^2}{v^2}}\right]\right\} \tag{11a}$$

$$F_-(t\mid x) = \delta\left(t-\frac{x}{v}\right)\mathrm{e}^{-kt} + \mathrm{H}\left(t-\frac{x}{v}\right)\frac{xk\mathrm{e}^{-kt}}{v\sqrt{t^2-x^2/v^2}}\,\mathrm{I}_1\left[k\sqrt{t^2-\frac{x^2}{v^2}}\right] \tag{11b}$$

where $\mathrm{I}_1[\cdots]$ is the modified Bessel function of order one.

It is of interest to examine some special cases of these general expressions. When $k=0$, $F_+(t\mid x)=0$ as to be expected since a particle moving with $+v$ can never be absorbed. In this limit, $F_-(t\mid x)=\delta(t-x/v)$ so that $S_-(t\mid x)=1-\mathrm{H}(t-x/v)$, i.e., the survival probability is one until time $t=x/v$ and zero thereafter. The distribution of first passage times for a particle starting out at $x=0$ but moving with velocity $+v$, from Eq. (11a), is $F_+(t\mid 0)=\mathrm{e}^{-kt}\mathrm{I}_1[kt]/t$ so that the corresponding survival probability is:

$$\begin{aligned} S_+(t\mid 0) &= 1-\int_0^t \mathrm{e}^{-k\tau}\frac{\mathrm{I}_1[k\tau]}{\tau}\,d\tau \\ &= \mathrm{e}^{-kt}\{\mathrm{I}_0[kt]+\mathrm{I}_1[kt]\} \end{aligned} \tag{12}$$

A particle starting out at $x=0$ with a velocity $+v$ can only be absorbed at $x=0$ if it changes its velocity to $-v$.

Let us examine the behavior of Eqs. (11a, 11b) at long times. When $t \gg x/v$ and $kt \gg 1$, using the asymptotic expansions of Bessel functions, $\mathrm{I}_0[y]=\mathrm{I}_1[y]\simeq[2\pi y]^{-1/2}\exp\{y\}$ for $y\to\infty$, and $y=k[t^2-(x/v)^2]^{1/2}\simeq kt-(kx^2)/(2v^2t)$, we find:

$$F_+(t\mid x) = \frac{(x+v/k)}{(4\pi Dt^3)^{1/2}}\exp\left[-\frac{x^2}{4Dt}\right] \tag{13a}$$

$$F_-(t\mid x) = \frac{x}{(4\pi Dt^3)^{1/2}}\exp\left[-\frac{x^2}{4Dt}\right] \tag{13b}$$

where we have defined $D=v^2/(2k)$. Note that the reduced distribution $F(t\mid x)=[F_+(t\mid x)+F_-(t\mid x)]/2$ reaches zero at $x=-v/2k$ and satisfies the radiation boundary condition,

$$D\left.\frac{\partial F}{\partial x}\right|_{x=0} = \kappa F(t\mid 0) \qquad \text{with} \quad \kappa = v \tag{14}$$

This defines the Milne lenght, $l = D/\kappa = v/(2k)$, for the diffusion limit of the telegrapher's equation or two velocities process. When in addition $kx/v \gg 1$, i.e., $F_+(t \mid x) = F_-(t \mid x)$ for sufficiently long times, $F(t \mid x)$ is just the first passage time distribution to an absorbing boundary for a freely diffusing particle with diffusion coefficient D, i.e., the solution of the Wang–Uhlenbeck problem in the diffusion limit. As a result of the above slow $[t^{-3/2}]$ asymptotic decay of the first passage time distribution functions, the mean first passage time is infinite for this problem.

Finally, we consider generalizations of the above model that corresponds to more sophisticated velocity finite difference approximations of the Kramers–Klein equation. Suppose that the velocity can fluctuate among $\pm v$, $\pm 3v$,..., $\pm(2n-1)\,v$ with dynamics described by the scheme:

$$-(2n-1)\,v \underset{k}{\overset{(2n-1)\,k}{\rightleftharpoons}} -(2n-3)\,v \underset{2k}{\overset{(2n-2)\,k}{\rightleftharpoons}} \cdots$$

$$\underset{(2n-2)\,k}{\overset{2k}{\rightleftharpoons}} (2n-3)\,v \underset{(2n-1)\,k}{\overset{k}{\rightleftharpoons}} (2n-1)\,v$$

Let $V_i = (2i - 2n - 1)\,v$ $[i = 1, 2,..., 2n]$ so that the above kinetic scheme can be relabeled as,

$$V_1 \underset{k}{\overset{(2n-1)\,k}{\rightleftharpoons}} V_2 \underset{k}{\overset{(2n-2)\,k}{\rightleftharpoons}} \cdots \underset{(2n-2)\,k}{\overset{2k}{\rightleftharpoons}} V_{2n-1} \underset{(2n-1)\,k}{\overset{k}{\rightleftharpoons}} V_{2n}$$

The probability, $p_{\text{eq}}(i)$, that at equilibrium the velocity is V_i is given by the binomial distribution:

$$p_{\text{eq}}(i) = \frac{1}{2^{2n}} \binom{2n-1}{i-1} = \frac{(2n-1)!}{2^{2n}(i-1)!\,(2n-i)!}; \qquad i = 1, 2,..., 2n \tag{15}$$

For this model, $\langle V^2 \rangle_{\text{eq}} = (2n-1)\,v^2$, and the velocity autocorrelation function is e^{-2kt} for all n.

Let $S_i(t \mid x)$ be the survival probability of a particle initially at x with velocity V_i. When $n = 1$, for instance, $S_1(t \mid x)$ and $S_2(t \mid x)$ correspond to $S_-(t \mid x)$ and $S_+(t \mid x)$ defined previously. The elements of the survival probability vector satisfy the following equation,

$$\frac{\partial S_i}{\partial t} = V_i \frac{\partial S_i}{\partial x} + (2n-i)\,kS_{i+1} - (2n-1)\,kS_i + (i-1)\,kS_{i-1}; \qquad i = 1, 2,..., 2n \tag{16}$$

which, after Laplace transformation, is analogous to Eq. (4) but where $\mathbf{M}$ is $2n \times 2n$ matrix with elements:

$$M_{ij} = -\frac{1}{(2i-2n-1)\,v}\begin{cases}(2n-i)\,k & \text{if } j=i+1\\ -(2n-1)\,k-\sigma & \text{if } j=i\\ (i-1)\,k & \text{if } j=i-1\\ 0 & \text{otherwise}\end{cases} \tag{17}$$

The eigenvalue problem, $\mathbf{Mu} = \lambda\mathbf{u}$, is equivalent to solving the difference equation:

$$(2n-i)\,ku_{i+1} - [\sigma + (2n-1)\,k + (2n+1-2i)\,\lambda v]\,u_i + (i-1)\,ku_{i-1} = 0 \tag{18}$$

Introducing the generating function,

$$G(y) = \sum_{i=1}^{2n} y^{i-1} u_i p_{\text{eq}}(i) \tag{19}$$

Eq. (18) leads to the first-order differential equation,

$$\frac{\partial G}{\partial y} - \left[\frac{(2n-1)\,ky - \sigma - (2n-1)\,k - (2n-1)\,\lambda v}{ky^2 - 2\lambda vy - k}\right] G = 0 \tag{20}$$

The general solution of this differential equation is

$$G(y) = C[y-y_1]^{\alpha}\,[y-y_2]^{\beta} \tag{21a}$$

$$\left.\begin{matrix}\alpha\\ \beta\end{matrix}\right\} = \frac{(2n-1)}{2} \mp \frac{[\sigma + (2n-1)\,k]}{2\sqrt{(\lambda v)^2 + k^2}} \tag{21b}$$

$$\left.\begin{matrix}y_1\\ y_2\end{matrix}\right\} = \frac{\lambda v \pm \sqrt{(\lambda v)^2 + k^2}}{k} \tag{21c}$$

where C is an arbitrary constant which can be set to one. Since $G(y)$ must be a polynomial of degree $2n-1$ in y, we require that $\beta - \alpha = 2i - 2n - 1$, with $1 \leqslant i \leqslant 2n$. From this condition, it turns out that the eigenvalues of the matrix $\mathbf{M}$ are:

$$\lambda_i = \frac{\sqrt{[\sigma + (2n-1)\,k]^2 - (2i-2n-1)^2\,k^2}}{(2i-2n-1)\,v}, \qquad i = 1, 2,..., 2n \tag{22}$$

in which $\lambda_i < 0$ for $1 \leqslant i \leqslant n$ and $\lambda_i > 0$ for $n \leqslant i \leqslant 2n$. The generating function corresponding to the eigenvalue λ_i:

$$G_i(y) = [y - y_1]^{2n-i}[y - y_2]^{i-1} = \sum_{j=1}^{2n} u_j^{(i)} y^{j-1}, \qquad j = 1, 2, ..., 2n \tag{23}$$

where $u_j^{(i)}$ represent elements of the eigenvector $\mathbf{u}^{(i)}$ associated to the eigenvalue λ_i, i.e., $\mathbf{u}^{(i)} = (u_1^{(i)}, u_2^{(i)}, ..., u_{2n}^{(i)})^T$. These eigenvectors are given by:

$$u_j^{(i)}(\sigma) = y_1^{2n-i+1} y_2^{i+j-1} \sum_{l=0}^{j-1} (-1)^l \binom{i-1}{l} \binom{2n-i}{j-l-1} y_1^{2l} \tag{24}$$

in which y_1 and y_2 are defined in Eq. (21c) with λ_i given by Eq. (22).

Consequently, the method used above for $n = 1$ can be easily generalized. The first passage time distribution vector can be written as:

$$\hat{\mathbf{F}}(\sigma \mid x) = \sum_{i=1}^{n} B_i \mathbf{u}^{(i)} e^{\lambda_i x}; \qquad \lambda_i < 0 \tag{25}$$

where $\mathbf{u}^{(i)}$ are eigenvectors corresponding to the negative eigenvalues. The B_i's can be determined from the n boundary conditions,

$$\hat{F}_j(\sigma \mid 0) = \sum_{i=1}^{n} B_i u_j^{(i)} = 1; \qquad j = 1, 2, ..., n \tag{26}$$

Equation (25), with the B_i's given in Eq. (26), constitutes the formal solution in the Laplace space of the Wang–Uhlenbeck problem in the discrete velocity space.

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REFERENCES

1. M. C. Wang and G. E. Uhlenbeck, *Rev. Mod. Phys.* **17**:323 (1945).
2. H. A. Kramers, *Physica* **7**:284 (1940); O. Klein, *Arkiv. Mat. Astr. Fys.* **16**:5 (1922); V. I. Melnikov, *Phys. Rep.* **209**:1 (1991).
3. T. W. Marshall and E. J. Watson, *J. Phys. A: Math. Gen.* **18**:3531 (1985); **20**:1345 (1987).
4. G. I. Taylor, *Proc. Lond. Math. Soc.* **20**:196 (1921).
5. S. Goldstein, *Quart. J. Mech. Appl. Math.* **4**:129 (1951).
6. J. Masoliver, J. Porrà, and G. H. Weiss, *Phys. Rev. A* **45**:2222 (1992) and **46**:3574 (1992); *Phys. Rev. E* **48**:939 (1993).
7. A. P. Prudnikov, Yu. A. Brychkov, and O. I. Marichev, *Integrals and Series* (Gordon and Breach Science Publishers, New York, 1992), Vol. 5, p. 61.

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