Drift and diffusion in periodic potentials: Upstream and downstream step times are distributed identically

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This note deals with one-dimensional diffusion of particles in the potential $U(x)=V(x)-Fx$, where $V(x)=V(x+L)$ is a periodic potential of period L and $F\geq 0$ is a uniform driving force. This problem arises when describing, for example, superionic conductors, Josephson tunneling junctions, rotations of dipoles in a constant field, and phase-locked loops.[1] One of the main results of this note concerns the distributions of time τ required for a particle to make a step of length L in the upstream and downstream directions. Counterintuitively, it turns out that the probability densities of these times, $\varphi_{\pm}(\tau)$, are identical,

$$\varphi_{+}(\tau)=\varphi_{-}(\tau)=\varphi(\tau), \tag{1}$$

i.e., the step time distribution is direction independent while the step probabilities, W_+ and W_-, strongly depend on the step direction. These probabilities are given by

$$W_{+}=\frac{1}{1+\exp(-\beta FL)}, \quad W_{-}=\frac{\exp(-\beta FL)}{1+\exp(-\beta FL)}, \tag{2}$$

independently of the presence of the periodic potential, where $\beta=1/(k_BT)$ with the standard notations k_B and T for the Boltzmann constant and absolute temperature. We derive the relations in Eqs. (1) and (2) and then use them to obtain the expressions for the effective drift velocity, v_{eff}, and diffusion coefficient, D_{eff}, that describe the coarse-grained motion of the particles at times which are much longer than the mean step time.

Expressions for v_{eff} and D_{eff} were first derived by Reimann *et al.*[2] by calculating the long-time behavior of the first two moments of the displacement, $\Delta x(t)=x(t)-x(0)$, and using the definitions, $v_{\text{eff}}=\lim_{t\to\infty}\langle\Delta x(t)\rangle/t$ and $D_{\text{eff}}=\lim_{t\to\infty}\{\langle[\Delta x(t)]^2\rangle-\langle[\Delta x(t)]\rangle^2\}/(2t)$. In this note we suggest a different approach, which exploits the fact that after making a step of length L the particle is exactly in the same situation as initially. Based on this fact we map the continuous particle dynamics onto a nearest neighbor asymmetric continuous time random walk (CTRW) between sites separated by distance L. Then we use some recent results for asymmetric CTRW (Ref. 3) to obtain expressions for v_{eff} and D_{eff}. Although our formulas for v_{eff} and D_{eff}, Eqs. (10) and (11), look differently from those derived in Ref. 2, their identity can be proved by straightforward but cumbersome manipulations. In spite of the fact that both our analysis and that in[2] are based on the first-passage-time statistics, there is a significant distinction between the two since the first passage times used below and in Ref. 2 are different. The former are the first passage times from a starting point x_0 to the two points located at $x_0\pm L$, while the latter is the first passage time from the starting point to the point located at x_0+L with no constraints on the particle motion in the negative direction from the starting point. We believe that the new approach, which is focused on the particle motion on the finite interval of length $2L$, has an important advantage. It can be easily generalized and used to study (both analytically and numerically) similar problems in higher dimensions, for example, drift and diffusion in tubes with periodically varying cross section.

Given an arbitrary set of discrete points $\{x_i\}$, $i=0,\pm 1,\pm 2,\ldots$, one can always map one-dimensional diffusive motion in a potential onto a nearest neighbor CTRW on this set. In general, this CTRW is nonseparable[4] in the sense that the random walk first decides whether it makes the next step in the positive or negative direction and then uses the corresponding distribution of the step time to determine the moment when it makes the step. The distributions of the step time from a given site in the positive and negative directions in the general case are different. The situation changes dramatically when the potential has the form $U(x)=V(x)-Fx$ with $V(x)=V(x+L)$ and the set $\{x_i\}$ is chosen so that $x_{i\pm 1}=x_i\pm L$. The reason is that in such a case, as follows from Eq. (1), the step time probability densities in both directions are identical. As a consequence, the CTRW becomes separable[4] in the sense that the random walk makes decisions about the moment when the next step is made and the step direction independently.

The CTRW is characterized by the step probabilities, $W_{\pm}$, and the step time probability densities, $\varphi_{\pm}(\tau)$. To derive $W_{\pm}$ in Eq. (2) consider a particle that starts from an arbitrary point x_0 at $t=0$ and is trapped at its first touch of one of the two end points located at x_L and x_R, $x_L<x_0<x_R$. The particle propagator, $G(x,t|x_0)$, considered as a function of x_0 satisfies the adjoint Smoluchowski equation,

$$\frac{\partial G}{\partial t}=e^{\beta U(x_0)}\frac{\partial}{\partial x_0}\left[D(x_0)e^{-\beta U(x_0)}\frac{\partial G}{\partial x_0}\right], \tag{3}$$

where $D(x)$ is the position-dependent diffusion coefficient, which is also a periodic function, $D(x+L)=D(x)$, the initial condition, $G(x,0|x_0)=\delta(x-x_0)$, and absorbing boundary conditions at the end points. The probability fluxes entering the trapping end points at time t are given by

$$f_L(t|x_0) = D(x_L)\frac{\partial G}{\partial x}\bigg|_{x=x_L}, \quad f_R(t|x_0) = -D(x_R)\frac{\partial G}{\partial x}\bigg|_{x=x_R}. \tag{4}$$

The probabilities of the particle trapping by the left (L) and right (R) end points, $W_{L,R}(x_0)$, are given by the time integrals of the fluxes, $W_{L,R}(x_0)=\int_0^\infty f_{L,R}(t|x_0)dt$. Based on the definitions above it can be shown that $W_{L,R}(x_0)$ satisfy

$$\frac{d}{dx_0}\left[D(x_0)e^{-\beta U(x_0)}\frac{dW_{L,R}(x_0)}{dx_0}\right]=0, \tag{5}$$

with the boundary conditions $W_L(x_L)=W_R(x_R)=1$, $W_L(x_R)=W_R(x_L)=0$. Solving Eq. (5) we find

$$W_L(x_0)=\frac{\int_{x_0}^{x_R} e^{\beta U(z)}\frac{dz}{D(z)}}{\int_{x_L}^{x_R} e^{\beta U(z)}\frac{dz}{D(z)}}, \quad W_R(x_0)=\frac{\int_{x_L}^{x_0} e^{\beta U(z)}\frac{dz}{D(z)}}{\int_{x_L}^{x_R} e^{\beta U(z)}\frac{dz}{D(z)}}. \tag{6}$$

Taking $x_L=x_0-L$, $x_R=x_0+L$ and using the fact that

$$\int_{x_0-L}^{x_0} e^{\beta U(z)}\frac{dz}{D(z)} = e^{\beta FL}\int_{x_0}^{x_0+L} e^{\beta U(z)}\frac{dz}{D(z)}, \tag{7}$$

we obtain the relations in Eq. (2). Note that the ratio of the probabilities W_+ and W_- given in Eq. (2) is equal to the ratio of the unbounded (unb) propagators $G_{\text{unb}}(x_0+L,t|x_0)$ and $G_{\text{unb}}(x_0-L,t|x_0)$, which satisfy Eq. (3) with absorbing boundaries moved to infinity, $W_+/W_-=G_{\text{unb}}(x_0+L,t|x_0)/G_{\text{unb}}(x_0-L,t|x_0)=\exp(\beta FL)$.

We next derive the identity of the step time probability densities, Eq. (1). To derive the identity we exploit the fact that any trajectory that starts from x_0 and is terminated at $x_0 \pm L$, consists of two parts, namely, the direct transition (dtr) part, which begins at x_0 and ends up at $x_0 \pm L$ without coming back to x_0, and the loop (l) part, which is the rest of the trajectory. Considering all trajectories terminated at x_0+L we can introduce probability densities for durations of the loop and direct transitions parts of such trajectories, $\varphi_+^{(l)}(\tau)$ and $\varphi_+^{(\text{dtr})}(\tau)$. Using these functions we can write $\varphi_+(\tau)$ as

$$\varphi_+(\tau)=\int_0^\tau \varphi_+^{(\text{dtr})}(\tau')\varphi_+^{(l)}(\tau-\tau')d\tau'. \tag{8}$$

Respectively, $\varphi_-(\tau)$ is given by

$$\varphi_-(\tau)=\int_0^\tau \varphi_-^{(\text{dtr})}(\tau')\varphi_-^{(l)}(\tau-\tau')d\tau', \tag{9}$$

where $\varphi_-^{(l)}(\tau)$ and $\varphi_-^{(\text{dtr})}(\tau)$ are defined using all trajectories trapped at x_0-L. It is obvious that $\varphi_+^{(l)}(\tau)=\varphi_-^{(l)}(\tau)$. The identity of the probability densities of the direct transition times, $\varphi_+^{(\text{dtr})}(\tau)=\varphi_-^{(\text{dtr})}(\tau)$, is a consequence of the theorem proved in Ref. 5 and the fact that $\varphi_+^{(\text{dtr})}(\tau)$ found for particles starting from x_0 and trapped at x_0+L is identical to $\varphi_+^{(\text{dtr})}(\tau)$ found for particles that start from x_0-L and are trapped at x_0. Thus, the identity of the probability densities $\varphi_+(\tau)$ and $\varphi_-(\tau)$ in Eq. (1) is a consequence of the identities of the probability densities of durations of the two parts of the trajectories.

We obtain v_{eff} and D_{eff} using the relations recently derived in Ref. 3

$$v_{\text{eff}}=(W_+-W_-)\frac{L}{\langle\tau\rangle}=\tanh\left(\frac{\beta FL}{2}\right)\frac{L}{\langle\tau\rangle} \tag{10}$$

and

$$\begin{aligned} D_{\text{eff}} &= \left[1+(W_+-W_-)^2\left(\frac{\langle\tau^2\rangle}{\langle\tau\rangle^2}-2\right)\right]\frac{L^2}{2\langle\tau\rangle} \\ &= \left\{1+\left[\tanh\left(\frac{\beta FL}{2}\right)\right]^2\left(\frac{\langle\tau^2\rangle}{\langle\tau\rangle^2}-2\right)\right\}\frac{L^2}{2\langle\tau\rangle}, \end{aligned} \tag{11}$$

where $\langle\tau^n\rangle=\int_0^\infty \tau^n\varphi(\tau)d\tau$ is the nth moment of the particle first passage time to one of the absorbing boundaries located at distances $\pm L$ from the particle starting point. The moments of the particle first passage time from x_0 to the absorbing boundaries located at x_L and x_R, $x_L<x_0<x_R$, $\langle t^n(x_0)\rangle$, satisfy

$$\frac{d}{dx_0}\left[D(x_0)e^{-\beta U(x_0)}\frac{d\langle t^n(x_0)\rangle}{dx_0}\right]=-ne^{-\beta U(x_0)}\langle t^{n-1}(x_0)\rangle, \tag{12}$$

with boundary conditions $\langle t^n(x_L)\rangle=\langle t^n(x_R)\rangle=0$. Solving Eq. (13) for $x_L=x_0-L$ and $x_R=x_0+L$ we obtain

$$\begin{aligned} \langle\tau\rangle &= \frac{1}{1+e^{-\beta FL}}\int_{x_0-L}^{x_0+L} e^{\beta U(z)}\frac{dz}{D(z)}\int_{x_0-L}^{z} e^{-\beta U(y)}dy \\ &\quad -\int_{x_0-L}^{x_0} e^{\beta U(z)}\frac{dz}{D(z)}\int_{x_0-L}^{z} e^{-\beta U(y)}dy \end{aligned} \tag{13}$$

and

$$\begin{aligned} \frac{\langle\tau^2\rangle}{2} &= \frac{1}{1+e^{-\beta FL}}\int_{x_0-L}^{x_0+L} e^{\beta U(z)}\frac{dz}{D(z)}\int_{x_0-L}^{z} e^{-\beta U(y)}\langle t(y)\rangle dy \\ &\quad -\int_{x_0-L}^{x_0} e^{\beta U(z)}\frac{dz}{D(z)}\int_{x_0-L}^{z} e^{-\beta U(y)}\langle t(y)\rangle dy, \end{aligned} \tag{14}$$

where the mean lifetime $\langle t(y)\rangle$ is given by

$$\begin{aligned} \langle t(y)\rangle &= \left[\int_{x_0-L}^{y} e^{\beta U(v)}\frac{dv}{D(v)}\right] \\ &\quad \times \frac{\int_{x_0-L}^{x_0+L} e^{\beta U(v)}\frac{dv}{D(v)}\int_{x_0-L}^{v} e^{-\beta U(u)}du}{\int_{x_0-L}^{x_0+L} e^{\beta U(v)}\frac{dv}{D(v)}} \\ &\quad -\int_{x_0-L}^{y} e^{\beta U(v)}\frac{dv}{D(v)}\int_{x_0-L}^{v} e^{-\beta U(u)}du. \end{aligned} \tag{15}$$

Substituting $\langle\tau\rangle$ and $\langle\tau^2\rangle$ given in Eqs. (13) and (14) into Eqs. (10) and (11) we obtain our final expressions for v_{eff} and D_{eff}.

Our results should be compared with the expressions for v_{eff} and D_{eff} derived in Ref. 2 by a different method. In Ref. 2 it was taken that $D(x)=\text{const}=D_0$ and found that $v_{\text{eff}}=L[1-\exp(-\beta FL)]/\int_{x_0}^{x_0+L}I_+(x)dx$ and $D_{\text{eff}}=L^2[\int_{x_0}^{x_0+L}I_+^2(x)I_-(x)dx]/[\int_{x_0}^{x_0+L}I_+(x)dx]^3$, where $I_\pm(x)=(1/D_0)\int_0^L\exp\{-\beta[\pm U(x)\mp U(x\mp y)]\}dy$. The identity of the results derived by the two methods can be checked by straightforward but cumbersome manipulations.

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