Analytical Solution to Transport in Brownian Ratchets via the Gambler's Ruin Model

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We present an analogy between the classic gambler's ruin problem and the thermally activated dynamics in periodic Brownian ratchets. By considering each periodic unit of the ratchet as a site chain, we calculated the transition probabilities and mean first passage time for transitions between energy minima of adjacent units. We consider the specific case of Brownian ratchets driven by Markov dichotomous noise. The explicit solution for the current is derived for any arbitrary temperature, and is verified numerically by Langevin simulations. The conditions for current reversal in the ratchet are obtained and discussed.

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In the *gambler's ruin* problem, a player plays a series of games against an adversary, winning (or losing) one dollar for every success (or failure), until one of them is "ruined." Given the probability of winning each game, the gambler's ruin problem considers the probability of ultimate ruin of one of the players, as well as the number of games required [1]. In this Letter, we show an intimate relationship between this classic random walk problem and the thermally activated dynamics in arbitrary potentials. The linkage between these two disparate topics is made possible by recent advances in the time quantification of Monte Carlo method [2,3]. In particular, the evolutionary techniques for the gambler's ruin problem can be utilized to analyze the transition probabilities and the mean first passage time (MFPT) of the complex stochastic transport in Brownian ratchets.

An oscillating driving force applied on Brownian particles in asymmetric periodic potentials (ratchets) can cause directed transport, i.e., imbalanced current [4–7]. The keen scientific interest in the transport property of Brownian ratchets is attributed to their role in biological systems, e.g., the astonishing energy-motion conversion of ATP hydrolysis [8]. One of the key questions in the study of Brownian ratchets is obtaining the expression for current. In general, the stochastic transport in the ratchets is modeled by Langevin equations of the form

$$\gamma \dot{x} = -U'(x, z(t)) + \xi(t), \tag{1}$$

where $\xi(t)$ is a mean-zero Gaussian white noise term, i.e., $\langle \xi(t)\xi(s)\rangle = 2\gamma k_B T \delta(t-s)$, and $z(t)$ is a Markov dichotomous process with correlation time τ_c. $\xi(t)$ represents the effects of thermal fluctuation, while $z(t)$ models stochastic processes such as impurities or defects jumping between metastable states [9]. The current is calculated by solving the corresponding Fokker-Planck equation under periodic boundary conditions. However, the explicit current expression can only be obtained for a few simple cases [9–11], due to the complexity of dichotomous processes induced dynamics. For nontrivial cases, the ratchet current can be calculated numerically either from the Langevin equation [12] or from the Fokker-Planck equation [13].

Numerical calculations are, however, computationally intensive and do not yield as much physical insight as analytical solutions. Thus, our objective is to derive the analytical expression of the ratchet current. Unlike previous methods, we based our technique on the Monte Carlo scheme, specifically the gambler's ruin model. Our analysis is presented in three main stages. (i) First, we justify the theoretical basis of using the Monte Carlo approach. This is done by establishing the time-quantification factor between a Monte Carlo step (MCS) and real time in seconds. (ii) Second, we formulate the Brownian ratchet problem in the Monte Carlo framework. (iii) Finally, by applying the evolutionary techniques in the gambler's ruin model, we analytically derive the expression of ratchets current for the thermal equilibrium case, and the more complex case of dichotomous noise.

Theoretical basis.—Time quantification of the MCS is most easily introduced by considering an overdamped Brownian particle in a steady potential $U(x, z(t)) = V(x)$. The random walk on x takes a fixed length trial move: $\Delta x = \pm R$ $(R \to 0)$ with equal trial probability in both directions but subject to the heat-bath acceptance rate of $1/[1 + \exp(\beta \Delta V)]$. Here ΔV is the energy difference in the proposed move and $\beta \equiv 1/k_B T$. Expanding the heat-bath acceptance rate, we obtain the mean μ and variance σ of Δx in *one* MCS: $\mu = -\frac{1}{4}\beta f(x) R^2$ and $\sigma^2 = \frac{1}{2}R^2 + O(R^4)$, where $f(x) = -V'(x)$ is the external force. Since $R \to 0$, the change of $f(x)$ within a few MCS is negligible. By the central limit theorem, after a large number n MCS the spread of displacement from x approximates the normal distribution:

$$P(\Delta x_{\rm MC}) = N(n\mu, n\sigma^2) = f(x) n\tfrac{1}{4}\beta R^2 + \eta\sqrt{2n\tfrac{1}{4}R^2}, \tag{2}$$

where $\eta \sim N(0, 1)$ follows the standard Gaussian distribution. We note that the integration form (Ito's interpretation) of the overdamped Langevin dynamical (LD) equation of Eq. (1) also results in a normal distribution of the displacement Δx after a time interval Δt_{LD}:

$$P(\Delta x_{\text{LD}}) = \frac{1}{\gamma} f(x)\Delta t_{\text{LD}} + \eta\sqrt{2(k_B T/\gamma)\Delta t_{\text{LD}}}. \quad (3)$$

Comparing Eqs. (2) and (3), we obtain a term-by-term equivalence between Δx_{MC} and Δx_{LD} if

$$1 \text{ MCS} = \Delta t_{\text{LD}}/n = \gamma\beta R^2/4. \quad (4)$$

Since the dichotomous process $z(t)$ simply produces transitions between two potential profiles [14], the equivalence established in Eq. (4) is still valid in the presence of $z(t)$, subject to the condition that $1 \text{ MCS} \ll \tau_c$. This equivalence justifies the use of Monte Carlo methods to analyze the ratchet current.

Problem formulation.—Macroscopically, the transport in L-periodic ratchets can be characterized as a series of successive "$\mathcal{L}$ transitions." An $\mathcal{L}$ transition is said to occur when a stochastic particle which is initially at x reaches an equivalent site a period away in either direction, i.e., $x + L$ or $x - L$, as shown in Fig. 1. Individually, an $\mathcal{L}$ transition can be analyzed as a classic random walk problem with absorbing boundaries. We define the forward transition probability as the probability of being absorbed to the right boundary $g \equiv p(x \to x + L)$ during the $\mathcal{L}$ transition. Conversely, the backward transition probability is defined as $h \equiv p(x \to x - L)$. Since the particle will ultimately reach either of the absorbing boundaries after a sufficiently long time, we have $g + h = 1$. The difference between g and h results in a nonzero current, and we thus have the steady current:

$$\langle \dot{x} \rangle := \lim_{t\to\infty} \frac{x(t) - x(0)}{t} = \frac{(g - h)L}{\tau_{\text{MFPT}}}, \quad (5)$$

where τ_{MFPT} is the MFPT for the particle starting at position x to hit either boundary at $x + L$ or $x - L$. τ_{MFPT} is a critical factor in describing the transport in the ratchets and has been studied for limited cases [11,15].

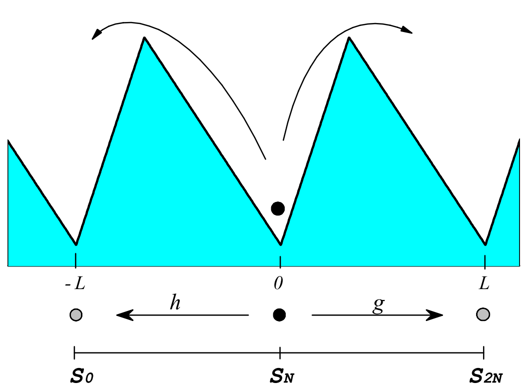

FIG. 1 (color online). Schematic diagram of an L-periodic ratchet potential.

Analytical solution for equilibrium case.—Based on Eq. (5), we require g, h, and τ_{MFPT} in order to obtain the current expression. We begin with a simple illustrative case—thermal equilibrium Brownian ratchets in the absence of a driven noise. We discretize the ratchets of length $2L$ into $2N + 1$ microsites so that positions of a particle take on a finite set of values $\{S_0, \ldots, S_{2N}\}$, as illustrated in Fig. 1. A particle starts at site S_m $(0 \le m \le 2N)$, and moves to adjacent microsites randomly, e.g., with steady probability μ_m to site S_{m-1} and with probability w_m to site S_{m+1} in one MCS. We define $g(m)$ as the probability that the particle starting at S_m reaches the absorbing site S_{2N} before it reaches the other absorbing site S_0 and $\tau(m)$ as the MFPT (in MCS) for the particle starting at S_m to reach either end site S_0 or S_{2N}. At the next MCS, the particle can either move to the left or right or stay put. According to the gambler's ruin problem [1],

$$g(m) = \mu_m g(m-1) + w_m g(m+1) + (1 - \mu_m - w_m)g(m), \quad (6)$$

$$\tau(m) = \mu_m \tau(m-1) + w_m \tau(m+1) + (1 - \mu_m - w_m)\tau(m) + 1. \quad (7)$$

The initial conditions $g(0) = 0$, $g(2N) = 1$, and $\tau(0) = \tau(2N) = 0$ apply.

The solution to the recurrence relation in Eq. (6) can be readily obtained. When $m = N$, we obtain the forward transition probability

$$g = g(N) = \frac{\sum_{i=0}^{N-1} k(i)}{\sum_{i=0}^{2N-1} k(i)} = \frac{1}{1 + k(N)}, \quad (8)$$

where $k(0) \equiv 1$, $k(m) \equiv \prod_{i=1}^{m} \mu_i/w_i$ for $m \ge 1$. In the last step we have used the periodic condition $\mu_j = \mu_{N+j}$ and $w_j = w_{N+j}$, which leads to $k(N + i) = k(N)k(i)$. The backward transition probability can be obtained from $h = (1 - g)$. Similarly from Eq. (7), for $m = N$,

$$\tau_{\text{MFPT}} = \tau(N) = g \sum_{i=1}^{N} \left[(w_i k(i))^{-1} \sum_{j=i}^{N+i-1} k(j) \right]. \quad (9)$$

Substituting the heat-bath rate definition $1/[1 + \exp(\beta\Delta V)]$ for w_i and μ_i into $k(i)$, we obtain $k(i) = (w_0/w_i)e^{\beta V_i} = 2w_0(e^{\beta V_i} + e^{\beta V_{i+1}})$, where V_i is the potential at the ith site and $V_0 \equiv 0$. Particularly, $k(N) = \exp(\beta V_N)$ since $w_0 = w_N$. Thus, by considering Eqs. (4) and (5), the current expression for ratchets in thermal equilibrium converges to the well-discussed continuous form [16,17] as $N \to \infty$:

$$\langle \dot{x} \rangle = \frac{(g - h)L}{\tau_{\text{MFPT}}} = \frac{L(1 - e^{\beta V(L)})}{\gamma\beta \int_0^L dx e^{-\beta V(x)} \int_x^{x+L} dy e^{\beta V(y)}}. \quad (10)$$

We shall also point out that for $N = 3$, our above discussion reduces to the three-state discrete-time minimal Brownian ratchet model [18].

Analytical solution for nonequilibrium case.—We now generalize our analysis to a nonequilibrium case, i.e., with an additional dichotomous noise $z(t)$ applied to the ratchets potential. We consider a mean-zero $z(t)$, which takes two discrete values $\{1, -\theta\}(\theta > 0)$ with correlation $\langle z(t)z(s)\rangle = \theta \exp(-|t-s|/\tau_c)$ [14]. For clarity, we denote "+" and "−" as representing the two states $z = 1$ and $z = -\theta$, respectively. Similar to our previous analysis, we define $g(m; \sigma; \sigma')$ as the probability for a particle at initial site S_m with $z(0) = \sigma$ to reach the absorbing site S_{2N} after some time t with $z(t) = \sigma'$ before it reaches the other absorbing site S_0. We also define $\tau(m; \sigma)$ as the MFPT for the particle starting at S_m under $z(0) = \sigma$ to reach any end sites. $g(m; \sigma; \sigma')$ can be generalized from Eq. (6),

$$g(m;\sigma;\sigma') = \sum_{\tilde{\sigma}=\pm} v(\tilde{\sigma}|\sigma)[w_m^{\tilde{\sigma}} g(m+1;\tilde{\sigma};\sigma') + \mu_m^{\tilde{\sigma}} g(m-1;\tilde{\sigma};\sigma') + (1 - w_m^{\tilde{\sigma}} - \mu_m^{\tilde{\sigma}}) g(m;\tilde{\sigma};\sigma')], \quad (11)$$

where $v(\tilde{\sigma}|\sigma)$ is the transition probability for dichotomous state from σ to $\tilde{\sigma}$ in *one* MCS [14]. $w_m^{\tilde{\sigma}}$ and $\mu_m^{\tilde{\sigma}}$ denote the spatial transition rates at dichotomous state $z = \tilde{\sigma}$. Equation (11) can be rewritten into a 2×2 matrix difference equation.

$$G_{m+1} = W_m^{-1}(\lambda C + W_m + U_m)G_m - W_m^{-1}U_m G_{m-1}, \quad (12)$$

where $\lambda \equiv v(-|+)/[1 - v(-|+) - v(+|-)] \ll 1$, $W_m = \mathrm{diag}\{w_m^+, w_m^-\}$, $U_m = \mathrm{diag}\{\mu_m^+, \mu_m^-\}$, and

$$C = \begin{pmatrix} 1 & -1 \\ -\theta & \theta \end{pmatrix}; \qquad G_m = \begin{pmatrix} g(m;+;+) & g(m;+;-) \\ g(m;-;+) & g(m;-;-) \end{pmatrix}.$$

We obtain the forward transition probability matrix by setting the starting position at $m = N$, i.e., $G = G_N$, and the boundary conditions as $G_0 = \mathbf{0}$; $G_{2N} = \mathrm{diag}\{1, 1\} \equiv I$. In the limit $N \to \infty$, $G = Q(L)[Q(2L)]^{-1}$, where $Q(y) = \{q(y;\sigma;\sigma')\}$ is a 2×2 matrix with $q(y;\sigma;\sigma')$ being defined as

$$\frac{\sigma\sigma'}{|\sigma\sigma'|} q(y;\sigma;\sigma') = \delta_{\sigma\sigma'} \int_0^y dx e^{\beta U(x,\sigma)} + \sum_{n=2}^{\infty} \left(\frac{\gamma\beta}{(1+\theta)\tau_c}\right)^{n-1} \Bigg[\sum_{\substack{\sigma_1=\sigma';\sigma_n=\sigma; \\ \text{other } \sigma_i=\pm}} \int_{x_0=0}^{x_n=y} \int_{x_0}^{x_{n-1}} \cdots \int_{x_0}^{x_2} dx_{n-1},\ldots,dx_1 \times \left(\prod_{j=2}^{n} |\sigma_j| \int_{x_{j-1}}^{x_j} dx e^{\beta[U(x,\sigma_j) - U(x_j,\sigma_j)]} \right) \int_{x_0}^{x_1} dx e^{\beta U(x,\sigma_1)} \Bigg]. \quad (13)$$

The backward transition probability matrix H can be calculated in a similar procedure as G.

Next, we generalize Eq. (7) for the MFPT function $\tau(m; \sigma)$ and obtain the matrix difference equation:

$$W_m T_{m+1} = (\lambda C + W_m + U_m)T_m - U_m T_{m-1} - E, \quad (14)$$

where $T_m = (\tau(m;+), \tau(m;-))^T$, $E = (1, 1)^T$, and $T_0 = T_{2N} = 0$. The explicit solution to the MFPT matrix $T = T_N$, as $N \to \infty$, has the form $T = GR(2L) - R(L)$ where the matrix $R(y) = (r(y;+), r(y;-))^T$, with $r(y;\sigma)$ given by

$$\frac{r(y;\sigma)}{\gamma\beta} = \sum_{n=2}^{\infty} \left(\frac{\gamma\beta}{(1+\theta)\tau_c}\right)^{n-2} \Bigg[\sum_{\substack{\sigma_{n-1}=\sigma; \\ \text{other } \sigma_i=\pm}} \int_{x_0=0}^{x_n=y} \int_{x_0}^{x_{n-1}} \cdots \int_{x_0}^{x_2} dx_{n-1},\ldots,dx_1 \frac{|\sigma|}{\sigma\sigma_1} \prod_{j=1}^{n-1} |\sigma_j| \int_{x_j}^{x_{j+1}} dx e^{\beta[U(x,\sigma_j) - U(x_j,\sigma_j)]} \Bigg]. \quad (15)$$

With the transition probabilities G, H and the MFPT T, the expression for the steady state current can be derived. We note $Z = G + H$ is the actual transition matrix for the probability distribution of dichotomous state over one $\mathcal{L}$ transition. Hence, the steady state (after $n \to \infty$ transitions) yields the following probabilities of the dichotomous states at the start of the $(n+1)$th $\mathcal{L}$ transition: $\mathrm{Prob}(z = 1) = Z_{21}/(Z_{12} + Z_{21})$ and $\mathrm{Prob}(z = -\theta) = Z_{12}/(Z_{12} + Z_{21})$. The effective forward transition probability is then given by the weighted sum $g_{\mathrm{eff}} = \sum_{\sigma,\sigma'} \mathrm{Prob}(z = \sigma) g(N; \sigma; \sigma')$, and similarly for h_{eff}. Based on Eq. (5), this leads to our main result, i.e., the analytical expression of the ratchets current in terms of the matrix elements of G, H, and T:

$$\langle \dot{x} \rangle = \frac{G_{11} + G_{22} - H_{11} - H_{22} - 2(|G| - |H|)}{(G_{21} + H_{21})T_1 + (G_{12} + H_{12})T_2} L. \quad (16)$$

For verification, we performed a numerical simulation based on the Langevin equation of Eq. (1), and assumed a ratchet potential profile of

$$U(x, z(t)) = \begin{cases} -\frac{1}{\hat{k}} L\hat{x} - z(t)Fx, & \hat{x} \le \hat{k}, \\ \frac{1}{1-\hat{k}} L\hat{x} - z(t)Fx, & \hat{x} > \hat{k}, \end{cases} \quad (17)$$

where $\hat{x} = x/L - [x/L]$, and $\hat{k} = 2/3$ reflects the asymmetry of the potential [9].

In Fig. 2, we plotted the particle current from the Langevin simulation and obtained extremely close agreement with the predictions of Eq. (16). We remark that recurring Eqs. (12) and (14) is a very efficient approach to calculate the G, H, and T to arbitrary precision as $N \to \infty$.

Asymmetry in potential profile and dichotomous fluctuations can result in current reversal [9]. The Monte Carlo method enables us to obtain precisely the vanishing current condition (see the inset of Fig. 2) which is of importance in rectifying particles with only small differences in γ.

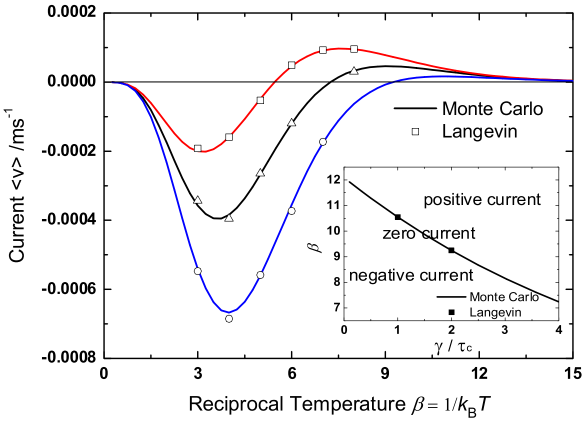

FIG. 2 (color online). Temperature-driven reversal of ratchets current. Close agreement between analytical Monte Carlo prediction and Langevin dynamical simulation. The simulation parameters are $R = 0.005$, $L = 1.0$, $F = 0.6$, $\theta = 0.42$, $\gamma = 1$, and $\tau_c = 0.15$, 0.25, 0.5 from top to bottom. Error bars are smaller than the symbol size. Inset: Extracted zero-current curve with respect to γ/τ_c.

Interestingly, since $\lambda \cong \Delta t/(1 + \theta)\tau_c = (\gamma/\tau_c) \times [\beta R^2/4(1 + \theta)]$, from Eq. (13) we found (γ/τ_c) determines the current direction. In Figs. 2 and 3, we observed two facts: (1) There is a threshold temperature β_c, below which no current reversal can occur regardless of γ and τ_c, and (2) the zero-current condition curve is *monotonic* in character, i.e., a decrease in the required γ/τ_c with increasing β. A qualitative explanation may be obtained by considering the energy barrier between the supersites ΔV^+, ΔV^- when the ratchet is tilted by the dichotomous noise $z = 1$ and $z = -\theta$, respectively. In the present application, $\Delta V^+ < \Delta V^-$, and hence a positive current occurs in the limit of high β. While at *low* β and *large* τ_c limit such that $\tau_{\mathrm{MFPT}} \ll \tau_c$, a negative current will be formed if $[\exp(-\beta\Delta V^+)/\theta] < \exp(-\beta\Delta V^-)$. Therefore, the bottom-left (top-right) corner of the phase diagram of Fig. 3 corresponds to a negative (positive) current region,

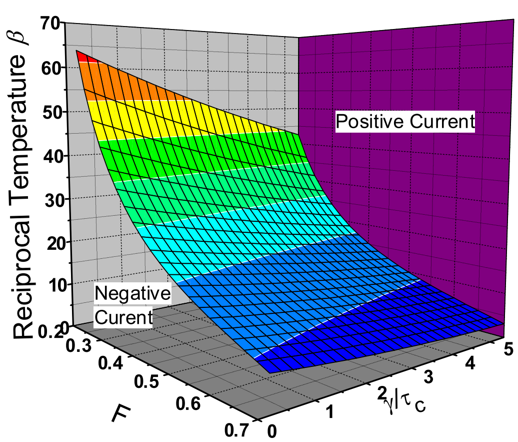

FIG. 3 (color online). The zero-current surface with respect to parameters β, γ/τ_c, and F.

thus implying a monotonic trend of the zero-current surface dividing the two regions.

Note that the analytical ratchet current in Eq. (16) is derived without the assumption of low temperature as in [11]. Additionally, for the specific case of $N = 2$, our discussion on ratchets transport in the presence of dichotomous process reduces to the minimal Astumian game [19]. Finally, the above Monte Carlo method can reasonably be extended to ratchets driven by an n-state process or even an Ornstein-Uhlenbeck (OU) process [16] (an OU process is equivalent to an infinite n-state process from the Monte Carlo point of view).

For detailed derivations of some of the results presented here, see the supplementary material in Ref. [20].

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[20] See EPAPS Document No. E-PRLTAO-99-032734 for detailed derivations of some of the results presented here. For more information on EPAPS, see http://www.aip.org/pubservs/epaps.html.