Escape from a fluctuating system: A master equation and trapping approach

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(Received 22 April 1999)

We present a general solution for the mean exit time in a system with on-site fluctuations between two configurations described by a master equation. The coupled configurations represent a spatially discretized version of an escape over a fluctuating barrier [C. R. Doering and J. C. Gadoua, Phys. Rev. Lett. **69**, 2318 (1992)], and passage through modulating channels. Based on the general properties of the mean exit time, we obtain a simple solution for a coupled ''birth'' and ''death'' case that exhibits resonant activation. Within this exactly solvable model we derive analytically the optimal fluctuating rate, which is sensitive to the initial condition and scales as $1/n$, where n is the system size. Our approach unifies a number of escape problems and points towards the generality of resonant activation. [S1063-651X(99)15808-2]

PACS number(s): 05.40.Ca, 82.20.Db, 82.20.Mj

Fluctuations that switch between two configurations of a given system are common to a broad range of dynamical problems and are usually modeled by a dichotomic Markovian noise. The question of interest in this problem of a modulating environment has been the mean time to exit the system, or to react. Examples for such processes are escape over a fluctuating potential barrier with linear [1,2], periodic [3], or double-well potentials [4], and a fluctuating potential given by a barrier that can be present or absent [5]. It has been demonstrated that under certain conditions the mean exit time (MET) has a minimum as a function of the switching rate, a phenomenon known as resonant activation [1–4,6]. Here we investigate the problem of the exit time in a model of two configurations $(+)$ and $(-)$ coupled by a symmetric Markovian dichotomous noise. The probabilities of occupying the $(+)$ and $(-)$ configurations are given by ρ_+ and ρ_-, respectively, which, in the absence of traps, obey

$$\frac{d}{dt}\begin{pmatrix}\rho_+\\ \rho_-\end{pmatrix}=\begin{pmatrix}-\gamma & \gamma\\ \gamma & -\gamma\end{pmatrix}\begin{pmatrix}\rho_+\\ \rho_-\end{pmatrix}. \tag{1}$$

This corresponds to the scheme $(+)\rightleftarrows(-)$, where γ is the switching rate between the two configurations. Each configuration has its own inherent kinetics which usually follows a Fokker-Planck equation [1–3], but which can also be given in terms of a master equation. In Fig. 1 we present schematically such coupled configurations with a trap, where the kinetics of configurations $(+)$ and $(-)$ are given by the matrices $\mathbf{A}_+$ and $\mathbf{A}_-$. The on-site fluctuation rate γ, $\gamma>0$, is time independent and the transition from the ith site in configuration $(+)$ takes place to the corresponding ith site in configuration $(-)$. Note that in the absence of traps the systems in Fig. 1 satisfy Eq. (1). The model is a spatially discretized version of the Doering-Gadoua model for escape over a fluctuating barrier [1]. Within the approach presented here one can make use of, and establish connections to, random walk results in finite one-dimensional systems. The relationship to random walk theories introduces additional calculation techniques and broadens the scope of problems where fluctuating environments can be considered. As we show, it allows for

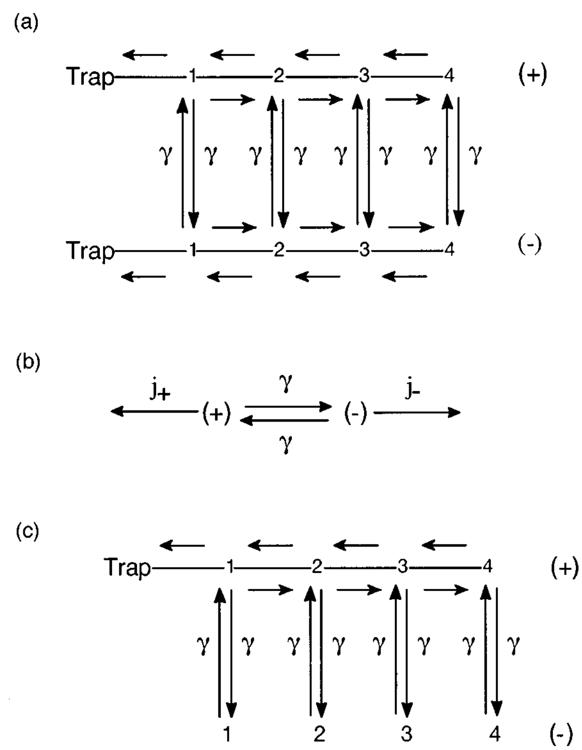

FIG. 1. (a) Example of a system that fluctuates between two configurations. The inherent kinetics in the upper configuration $(+)$ is given by matrix $\mathbf{A}_+$, and in the lower configuration $(-)$ by $\mathbf{A}_-$. The arrows within each configuration represent the intraconfigurational kinetics. The trap location corresponds to site 0. (b) Two coupled configurations represented by two sites. Note that such a system does not display resonant activation. (c) Two coupled configurations $(+)$ and $(-)$, where the $(-)$ configuration does not allow for motion.

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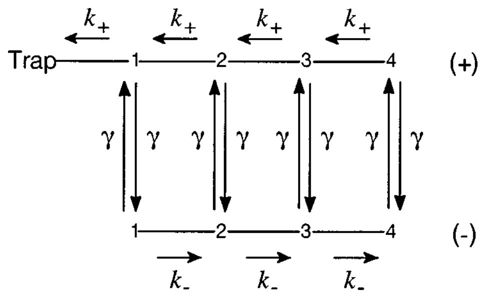

FIG. 2. Schematic representation of the coupled ''birth'' and ''death'' process.

an analytical solution of the ''birth'' and ''death'' problem in Fig. 2, and raises the possibility of resonant activation in other systems of modulating environments, such as ionic channels with flipping voltage [7] and molecular passage through a stochastic open-or-closed gate [5,8].

In what follows we consider the case that at least one of the configurations includes a trap at the origin, which is responsible for the exiting process, and a continuous path from each site to the trap. This guarantees that the corresponding matrix has an inverse and therefore a finite MET for any initial condition [9]. We study some general properties of the MET in the case where the intraconfiguration kinetics are described in terms of a master equation, and introduce a ''birth'' and ''death'' kinetic model that has an analytical solution that displays a resonant activation and it dependence on the system size and rates. We also introduce a relationship between the MET of the system and the stationary solution. For simplicity we use the following notations: a bold capital letter represents a matrix, and a capital letter represents a vector. The master equation that governs the systems in Fig. 1 is

$$\frac{d}{dt}\begin{pmatrix} P_+(t) \\ P_-(t) \end{pmatrix} = \begin{pmatrix} \mathbf{A}_+ - \gamma & \gamma \\ \gamma & \mathbf{A}_- - \gamma \end{pmatrix} \begin{pmatrix} P_+(t) \\ P_-(t) \end{pmatrix}, \tag{2}$$

where $P_+(t)$ and $P_-(t)$ are n-dimensional vectors of the probabilities to be at time t at the ith site of configurations $(+)$ and $(-)$, respectively. The $n \times n$ matrices $\mathbf{A}_+$ and $\mathbf{A}_-$ represent the kinetics of the corresponding configurations (note that the trap at site 0 is not included in the matrix representation). The total system is represented by a $2n \times 2n$ matrix. The survival probability within the coupled system is

$$\Phi(t) = \sum_{i \neq \text{trap}} p_+(i,t) + \sum_{i \neq \text{trap}} p_-(i,t), \tag{3}$$

where $p_+(i,t)$ and $p_-(i,t)$ are the ith elements of $P_+(t)$ and $P_-(t)$ respectively. The probabilities to be at the $(+)$ or $(-)$ configurations are

$$\rho_+ = \sum_{i \neq \text{trap}} p_+(i,t), \quad \rho_- = \sum_{i \neq \text{trap}} p_-(i,t). \tag{4}$$

The underlying process is basically a trapping process in a finite system [9,10]. The MET from the system, $\langle m \rangle$, is the time integral of the survival probability in Eq. (3) [9], and is given by

$$\langle m \rangle = \int_0^\infty \Phi(t)\,dt. \tag{5}$$

In order to calculate the MET we need to find the mean residence time which is the mean time spent by a walker on a site of the corresponding configuration prior to exiting (trapping). Taking the second time derivative of Eq. (2) we obtain, after rearrangement,

$$\ddot{P}_+(t) = (\mathbf{A}_+ + \mathbf{A}_- - 2\gamma)\dot{P}_+(t) + [\gamma(\mathbf{A}_+ + \mathbf{A}_-) - \mathbf{A}_-\mathbf{A}_+]P_+(t), \tag{6}$$

$$\ddot{P}_-(t) = (\mathbf{A}_+ + \mathbf{A}_- - 2\gamma)\dot{P}_-(t) + [\gamma(\mathbf{A}_+ + \mathbf{A}_-) - \mathbf{A}_+\mathbf{A}_-]P_-(t), \tag{7}$$

where the dots represent time derivatives. Laplace transforming Eqs. (6) and (7) $[\text{Laplace}[g] = \int_0^\infty e^{-st} g(t)\,dt]$ and substituting $s=0$, we obtain

$$M_+ = -[\gamma(\mathbf{A}_+ + \mathbf{A}_-) - \mathbf{A}_-\mathbf{A}_+]^{-1}[(\gamma - \mathbf{A}_-)P_+(0) + \gamma P_-(0)], \tag{8}$$

$$M_- = -[\gamma(\mathbf{A}_+ + \mathbf{A}_-) - \mathbf{A}_+\mathbf{A}_-]^{-1}[(\gamma - \mathbf{A}_+)P_-(0) + \gamma P_+(0)], \tag{9}$$

which are the vectors of the mean residence times in the configurations $(+)$ and $(-)$. Normalization of the initial condition satisfies $U[P_+(0) + P_-(0)] = 1$, where U is the n-dimensional summation vector $U = [1,1,1,1,1, \ldots, 1]$. Summing all the elements of the vectors M_+ and M_- yields the MET $\langle m \rangle$ of the coupled system [9],

$$\langle m \rangle = U(M_+ + M_-). \tag{10}$$

The vectors M_+ and M_- in Eqs. (8) and (9) are central in the calculation of the MET. The existence of the inverse matrices in Eqs. (8) and (9) stems from the existence of the inverse of $\mathbf{A}_+$ [11] which, as mentioned earlier, is guaranteed by the trap and the continuous path to the trap. The asymptotic values of the MET when starting at the reflecting points of the two configurations $P_+(0) = P_-(0) = P(0) = [0,0, \ldots, 0,0.5]^T$, are

(a) For the case of $\gamma \to 0$,

$$\langle m_{\gamma \to 0} \rangle = (\langle m_+ \rangle + \langle m_- \rangle)/2, \tag{11}$$

where $\langle m_+ \rangle, \langle m_- \rangle$ are the METs of the $(+)$ and the $(-)$ configurations correspondingly. Equation (11) is valid since the MET in a continuous Markov chain is a continuous function [12]. Note that if the MET of one of the configurations diverges, then the MET for the case of $\gamma \to 0$ diverges. If both configurations have an inverse transition matrix then we can rewrite Eq. (11) as

$$\langle m_{\gamma \to 0} \rangle = -U(\mathbf{A}_+^{-1} + \mathbf{A}_-^{-1})P(0), \tag{12}$$

which can be derived by letting $\gamma \to 0$ in Eqs. (8) and (9).

(b) For $\gamma \to \infty$ in Eqs. (8) and (9) we obtain the MET [7]

$$\langle m_{\gamma\to\infty}\rangle = -2U\left(\frac{\mathbf{A}_+ + \mathbf{A}_-}{2}\right)^{-1} P(0). \tag{13}$$

When $\gamma\to\infty$ the MET reduces to the calculation of the MET for a system with an average operator, which means that the probability to be at the ith site in the $(+)$ configuration is equal to the probability to be in the ith site in the $(-)$ configuration; namely, $\lim_{\gamma\to\infty} p_+(i,t) = p_-(i,t)$. Substituting this condition into Eq. (2) we recover Eq. (13) for the MET. This result recovers earlier results of the MET for a fast switching rate [1,2]. We now present two examples for applying the above framework. Let us first assume that $\mathbf{A}_+$ and $\mathbf{A}_-$ are 1×1 matrices,

$$\mathbf{A}_+ = -j_+, \quad \mathbf{A}_- = -j_-. \tag{14}$$

The model then reduces to the case of fluctuations between two sites, as shown in Fig. 1(b), which leads to the following MET, when starting at both sites:

$$\langle m\rangle = \frac{4\gamma + j_+ + j_-}{2[\gamma(j_+ + j_-) + j_+ j_-]}. \tag{15}$$

This concurs with a previous result [1,13]. This model does not have a minimum in the MET as a function of γ, since Eq. (15) is a monotonically decreasing function of γ. Another example, shown in Fig. 1(c), is that of configuration $(+)$ having a trap, but there is no motion along configuration $(-)$ so that $\mathbf{A}_- = \mathbf{0}$. From Eqs. (8) and (9) and for the initial condition of $P_+(0) = P_-(0) = P(0)$ we obtain

$$\langle m\rangle = -4UA_+^{-1}P(0) + (1/\gamma)UP(0). \tag{16}$$

Here again there is no minimum in the MET as a function of γ and the minimal MET is obtained for $\gamma\to\infty$.

An interesting relationship can be established between the MET and the stationary solution of the system. We consider the same system as described in Fig. 1, but with only one trap at the $(+)$ configuration and denote the rate from site 1 in the $(+)$ configuration to the trap by c. We distinguish between $\mathbf{W}$, the $2n\times 2n$ matrix representation of the whole system, and $\mathbf{W}_0$ the matrix for the stationary system, which does not have a trap. The relationship between the two systems is

$$\mathbf{W} = \mathbf{W}_0 + \begin{pmatrix} -c & 0 & 0... & 0 \\ 0 & 0 & 0... & 0 \\ \dots & \dots & \dots & 0 \\ 0 & 0 & 0... & 0 \end{pmatrix}. \tag{17}$$

Here we will show that $\mathbf{W}^{-1}Q(0)$ is a stationary solution of $\mathbf{W}_0$, where $Q(0) = [1,0,0,0,\dots,0]^T$. Consider a stationary solution X, namely, $\mathbf{W}_0 X = 0$, where $X = [x_1, x_2, \dots, x_N]^T$ and $\Sigma x_i = 1$. If X is the stationary solution, then also $X/(cx_1)$ is a stationary solution (without normalization).

Since $\mathbf{W}X/(cx_1) = Q(0)$, it follows that

$$X = (cx_1)\mathbf{W}^{-1}Q(0). \tag{18}$$

Therefore, calculating the vector of mean residence times of a random walker that starts at site 1 of the $(+)$ configuration, $\mathbf{W}^{-1}Q(0)$, yields the vector of the occupation probability of the system represented by $\mathbf{W}_0$. The normalization of the stationary solution is obtained by summing all the elements of the vector of mean residence times, namely, by calculating the MET with the initial condition $Q(0)$,

$$\langle m\rangle = UW^{-1}Q(0) = 1/(cx_1). \tag{19}$$

Note that this result yields $x_1 = 1/(c\langle m\rangle)$. This means that the maximum occupation probability at equilibrium of the nearest site to the trap is obtained when the MET starting at this site is minimal.

We now consider two coupled configurations as shown in Fig. 2. The $(+)$ one, described by $\mathbf{A}_+$, is a ''death'' process with a rate constant k_+, and the $(-)$ one is a ''birth'' process, described by $\mathbf{A}_-$, with a rate constant k_-. We will show that the coupled ''birth'' and ''death'' processes can be mapped onto a Markovian one-dimensional system. For this model we obtain analytically the optimal switching rate to escape from the system as a function of the size and the rates of the system. The matrix representation of the system is

$$\mathbf{A}_+ = \begin{pmatrix} -k_+ & k_+ & 0 & 0 & 0 \\ 0 & -k_+ & k_+ & 0 & 0 \\ 0 & 0 & -k_+ & .. & 0 \\ 0 & 0 & 0 & .. & k_+ \\ 0 & 0 & 0 & .. & -k_+ \end{pmatrix},$$

$$\mathbf{A}_- = \begin{pmatrix} -k_- & 0 & 0 & 0 & 0 \\ k_- & -k_- & 0 & 0 & 0 \\ 0 & k_- & -k_- & .. & 0 \\ 0 & 0 & k_- & .. & 0 \\ 0 & 0 & 0 & .. & 0 \end{pmatrix}. \tag{20}$$

In order to calculate the MET, starting at the reflecting point, we need to find the inverses matrices of $\gamma(\mathbf{A}_+ + \mathbf{A}_-) - \mathbf{A}_-\mathbf{A}_+$, and of $\gamma(\mathbf{A}_+ + \mathbf{A}_-) - \mathbf{A}_+\mathbf{A}_-$. Using Eq. (20) we obtain

$$\gamma(\mathbf{A}_+ + \mathbf{A}_-) - \mathbf{A}_-\mathbf{A}_+ = \begin{pmatrix} -q-r & l & 0 & 0 & 0 \\ r & -l-r & l & 0 & 0 \\ 0 & r & -l-r & l & 0 \\ 0 & 0 & r & \dots\dots & l \\ 0 & 0 & 0 & \dots\dots & -l \end{pmatrix} \tag{21}$$

and

$$\gamma(\mathbf{A}_+ + \mathbf{A}_-) - \mathbf{A}_+\mathbf{A}_- = \begin{pmatrix} -l-r & l & 0 & 0 & 0 \\ r & -l-r & l & 0 & 0 \\ 0 & r & -l-r & l & 0 \\ 0 & 0 & r & \dots\dots & q \\ 0 & 0 & 0 & \dots\dots & -q \end{pmatrix}, \tag{22}$$

where $r = k_+k_- + \gamma k_-$, $l = k_+k_- + \gamma k_+$, and $q = \gamma k_+$. The corresponding initial conditions for the matrices in Eqs. (21)

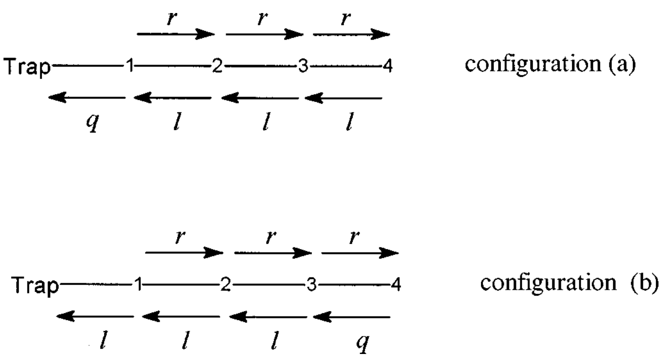

FIG. 3. One-dimensional representation of the matrices in Eqs. (21) and (22).

and (22) starting at the reflecting points $P(0)=P_+(0)=P_-(0)=[0,0,0,\ldots,0,0.5]^T$ are

$$(\gamma-\mathbf{A}_-)P_+(0)+\gamma P_-(0)=\gamma[0,0,0,\ldots,1]^T, \quad (23)$$

$$(\gamma-\mathbf{A}_+)P_-(0)+\gamma P_+(0)$$
$$=\gamma[0,0,0,\ldots,1]^T+\frac{k_+}{2}[0,0,0,\ldots,-1,1]^T. \quad (24)$$

The matrices in Eqs. (21) and (22) correspond to new one-dimensional configurations (a) and (b), respectively, shown in Fig 3. The problem of finding the MET is mapped onto the problem of finding the MET of configuration (a), $\langle m_a\rangle$, and the MET of configuration (b), $\langle m_b\rangle$, where each configuration describes a nearest neighbor jump process with the initial conditions given by Eqs. (23) and (24). The METs for starting at the reflecting are the same [9]; namely, $\langle m_a\rangle=\langle m_b\rangle$ and given for the general case $k_+\neq k_-$ by

$$\langle m_a\rangle=\frac{n+k_-/\gamma}{\gamma(k_+-k_-)}+\frac{k_-(k_++\gamma)}{\gamma^2(k_+-k_-)^2}\left[\frac{k_-}{k_+}\left(\frac{r}{l}\right)^{n-1}-1\right], \quad (25)$$

and for $k_+=k_-=k$ by

$$\langle m_a\rangle=\frac{n}{\gamma k}+\frac{n(n-1)}{2k(k+\gamma)}, \quad (26)$$

where n is the size of the system. Configuration (b) has an additional term in the initial condition $k_+/2[0,0,0,\ldots,-1,1]^T$, [Eq. (24)], which contributes $1/2\gamma$ to the MET [14]. The MET is therefore

$$\langle m\rangle=2\gamma\langle m_a\rangle+1/2\gamma. \quad (27)$$

Using Eq. (27) together with Eq. (26) we examine the possibility for resonant activation. We obtain the value of γ for the minimal MET by $d\langle m\rangle/d\gamma=0$, which for the case of $k_+=k_-=k$ leads to

$$\gamma_0=\frac{k}{\sqrt{2n(n-1)}-1}, \quad (28)$$

where we denote the extreme value of γ by γ_0. Taking the second derivative of Eq. (27) we find that it is a minimum

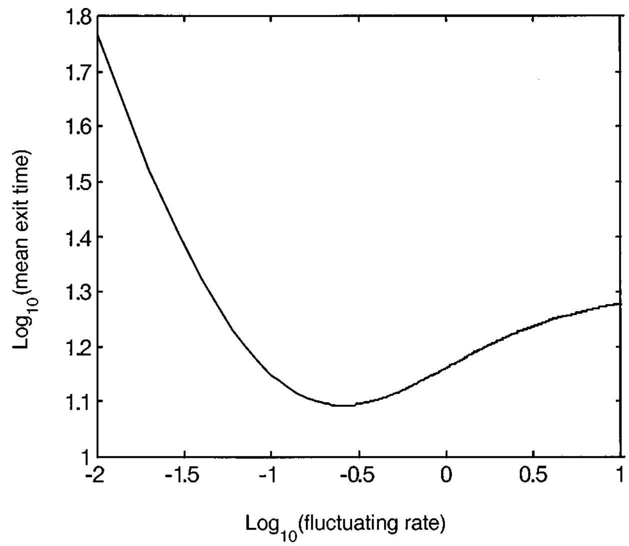

FIG. 4. Log_{10} (mean exit time) vs $\log_{10}$ (fluctuating rate) in dimensionless unit. Here $k=1$ and $n=4$. Resonant activation is obtained for $\gamma=\gamma_0$.

point. Such a minimum exists only for configurations of size $n>1$. The phenomenon of resonant activation is found also for the more general case of $k_+\neq k_-$. In Fig. 4 we plot the MET as a function of γ for the case of $n=4$. The MET when $\gamma\to 0$ is $\langle m_{\gamma\to 0}\rangle\to\infty$, since the MET of configuration $(-)$ is infinite. Substituting $\gamma\to\infty$ in Eqs. (26) and (27) we obtain $\langle m_{\gamma\to\infty}\rangle\to n(n+1)/k$, which is typical of MET for a symmetric random walk. The optimal MET, according to Eq. (28), is $\langle m_{\gamma=\gamma_0}\rangle=[2n+\sqrt{2n(n-1)}-0.5]/k$ which scales linearly with the system size for a large systems. In order to find the stationary solution, without the trap, in the ''birth''-''death'' case, Fig. 2, we calculate the MET of configurations (a) and (b) with the initial conditions $P_+(0)=[1,0,0,\ldots,0]^T$ and $P_-(0)=[0,0,0,\ldots,0]^T$. Solving for the MET in configuration (a), using Eqs. (8) and (9), we obtain the occupation probabilities at equilibrium for the $(+)$ configuration,

$$p_+(1,\infty)=1/(k_+\langle m\rangle),$$
$$p_+(i,\infty)=p_+(1,\infty)\gamma(r/l)^{i-1}/(\gamma+k_+), \quad i>1, \quad (29)$$

where the MET of the whole system in the case of $k_+\neq k_-$,

$$\langle m\rangle=2[(k_-/k_+)(r/l)^{n-1}-1]/(k_--k_+). \quad (30)$$

Note that the equilibrium states depend on the fluctuation rates. We see that a maximum in the occupation probability $p_+(1,\infty)$, Eq. (29) is reached when the MET is minimal.

In summary, we have presented a simple discrete formalism of a random walker in a modulating environment. The modulating environment can represent either switching between two different configurations, or, for example, the case where there is no change in configuration except for a single location which switches between absorbing and reflecting boundary conditions, mimicking an on-off gate. The kinetics of the walker in each configuration is described by a transition matrix. We have introduced an exactly solvable model which displays resonant activation when each configuration has more then one site. The analytically obtained minimum in the MET scales with system size as $1/n$ for large systems.

We thank Orr Ravitz for helpful discussions. J. K. acknowledges the support of the German Israeli Foundation (GIF) and a TMR European network grant (SISITOMAS).

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