The dynamical properties of a tracer repeatedly colliding with heat bath particles can be described within a Langevin framework provided that the tracer is more massive than the bath particles, and that the collisions are frequent. Here we consider the escape of a particle from a potential well, and the diffusion coefficient in a periodic potential, without making these assumptions. We have thus investigated the dynamical properties of a Stochastically Driven particle that moves under the influence of the confining potential in between successive collisions with the heat bath. In the overdamped limit, both the escape rate and the diffusion coefficient coincide with those of a Langevin particle. Conversely, in the underdamped limit the two dynamics have a different temperature dependence. In particular, at low temperature the Stochastically Driven particle has a smaller escape rate, but a larger diffusion coefficient.
Figure 1. Typical trajectories of the Stochastically Driven particle (left) and of the Brownian particle (right), for $\omega_0 t_c$ and $(\gamma/\omega_0)^{-1}$ equal to $10^{-1}$, $10^1$, $10^2$ at $T/\Delta U = 0.21$.

We have determined the escape rate and the diffusion coefficient in both the overdamped, $t_c \ll \tau_{cross}$, and the underdamped limits, $t_c \gg \tau_{cross}$, validating our theoretical results against numerical simulations and highlighting qualitative and quantitative differences with respect to the Langevin dynamics. In Fig. 1 we illustrate typical trajectories of the Stochastically Driven and of the Langevin dynamics, in the overdamped and the underdamped limits. In both cases the trajectories of the two dynamics appear qualitatively similar. However, we will show that only in the overdamped limit the two dynamics quantitatively agree. Indeed, in the underdamped limit the two dynamics differ, the Langevin one having an higher escape rate but, surprisingly, a smaller diffusion coefficient. This clarifies that the Brownian model is not appropriate in the underdamped limit to describe a physical system where the interaction with the heat bath occurs via successive collisions rather than via a continuous interaction.

Results

Escape rate. The escape rate is conventionally defined as the rate with which a particle “irreversibly” escapes from a well in a given direction. In a one dimensional periodic potential, the notion of irreversibility is easily clarified. A barrier crossing event is irreversible if it is not correlated to the subsequent one. Thus, an irreversible barrier crossing event is followed with probability 1/2 by a barrier crossing that brings the particle back to its original well, and with probability 1/2 by a barrier crossing event that brings the particle to the following well. To estimate the escape rate, we consider that the physical process leading to an irreversible escape comprises different steps. First, starting from thermal equilibrium, a particle performs a barrier crossing jump entering the arrival well. We indicate with $P_{\cap}$, its probability. Then, the particle performs different jumps remaining localized close to the top of the barrier, possibly crossing the top of the barrier a number of times. We indicate with $P\cap$ the probability that the particles crosses the barrier an even number of times, so that it remains in the arrival well. Finally, the particles moves away from the top of the barrier decorrelating in the arrival well, without the occurrence of any further recrossing. We call $P_d$ this probability. The escape rate is then given by $\Gamma_{SD} = P_{\cap} P_d (2 t_c)$. Since the probability that a particle recrosses a barrier an even number of times is $p = \sum_{n=0}^{\infty} P_d (1 - P_d)^n = (2 - P_d)^{-1}$, one finally gets

$$\Gamma_{SD}(t_c) = \frac{P_{\cap}(t_c) P_d(t_c)}{2t_c (2 - P_d(t_c))}. \tag{1}$$

To estimate the escape rate, we thus need to estimate the barrier crossing probability $P_{\cap}(t_c)$, and the decorrelating probability $P_d$. $P_{\cap}$ is obtained from an equilibrium average over the jumps. Indeed, each jump is characterized by three variables, the coordinate of the starting point, $x_s$, the initial velocity $v_s$, and the time of flight $t$. By the Boltzmann and Maxwellian equilibrium distribution, respectively, while $t$ is exponentially distributed with time constant $t_c$. Alternatively, each jump can be characterized by $x_s$, by the coordinate of the final point, $x_e$, and by the total energy $E$. Assuming with no loss of generality $|x| < L/2$, $P_{\cap}$ is the probability that $|x_e| > L/2$, which is found to be $P_{\cap} = \int_{-L/2}^{L/2} dx_s \int_{-L/2}^{L/2} dx_e \int_0^\infty dE f(x_s, x_e, E)$, where

$$f = \frac{1}{Z(T) \nu(x_s, E) \nu(x_e, E) t_c^{3/2} \pi^{3/2} m T}. \tag{2}$$

Here $f(x_s, x_e, E)$ is the probability that the walker interacts with the heat bath when in position $x_s$, through that interaction it acquires a total energy $E$, and that its flight time equals the time needed to travel from $x_s$ to $x_e$ with total energy $E$, which is given by $t_f (x_s \rightarrow x_e) = \int_{x_s}^{x_e} \frac{dx}{\nu(x, E)}$. $Z = \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} \int_0^\infty e^{-\frac{V(x_s, x_e, E)}{kT}} dE dx_s dx_e$ is a temperature dependent normalization constant. The predicted dependence of $P_{\cap}$ on $t_c$ illustrated in Fig. 2a (full line) correctly describes the numerical results. The high and small $t_c$ limits can be rationalized. In the $t_c \rightarrow 0$ limit, the above triple integral can be carried out, and one finds $P_{\cap} = \omega_0 t_c \nu^{-1} \nu^{-1} \nu^{-1} \exp(-\Delta U/T)$. In the $t_c \rightarrow \infty$ limit all jumps with enough energy cross the barrier and $P_{\cap}$ approaches a constant, whose weak temperature dependence is neglected in the following.
The decorrelation probability $P_d$ is estimated considering that, if a particle reaches a position which is at a far enough distance $l_t$ from the top of the barrier, then it decorrelates as its dynamics becomes dominated by the potential. We assume $l_t$ to be the distance at which the potential significantly affects the velocity $v(x, E) = \sqrt{(2m)(E - V(x))}$ of a particle crossing the barrier with energy $E$, and estimate $l_t \approx \sqrt{\Delta T/m\omega^2}$ through a Taylor expansion of $v(x, E)$ around the top of an energy barrier. In the overdamped limit $\omega t_c \ll 1, P_d$ is given by the probability that a barrier crossing event is followed by a sequence of jumps (of typical size $\xi$) able to drive the particle at distance $l_t \approx \sqrt{T}$ from the top, before a recrossing occurs. It is easy to show in a mean first passage time formalism\(^{18}\) that in this regime $P_d(t_c) \approx 2\omega t_c^2 \xi$. In the underdamped limit, $\omega t_c \gg 1$, jumps are long and barrier crossing events can be considered irreversible, so that $P_d = 1$. The numerical measure of $P_d(t_c)$ confirms our predictions for the overdamped and underdamped limits of $P_d$, as illustrated in Fig. 2b. We approximate in the following $P_d$ by a simple functional form able to capture the crossover between the $\omega t_c \ll 1$ and the $\omega t_c \gg 1$ limits, $P_d(t_c) = \frac{2\omega t_c^2}{\xi^2 + 2\omega t_c^2 \xi}$. We fix $k = \omega b/\omega_c$ exploiting an analogy with the Langevin dynamics in the overdamped low temperature limit, we will detail below.

Having determined $P_d(t_c)$ and $P_d(t_c)$, we can compute the escape rate $\Gamma(t_c)$ at all $t_c$ through Eq. 1. The overdamped and the underdamped limits result $\Gamma_{SD} = (1/2)\omega b \pi^{-1} (\omega t_c^2) e^{-\Delta U/T}$ and $\Gamma_{SD} \propto t_c^{-1} e^{-\Delta U/T}$, respectively. Figure 3 shows that our theoretical prediction (full line) well compares with numerical simulations of the model (open squares), at all $t_c$. In the figure, we also illustrate numerical results (full circles) for the escape rate of the Langevin dynamics, $\Gamma_L$. We remind that in the high damping regime, and in the low temperature limit, $\Gamma_L$ is the celebrated Kramers' escape rate\(^{19}\), $\Gamma_L = \frac{\omega b}{2\pi} \left[ 1 + \frac{\omega b}{4\omega_c^2} - \frac{\omega b}{2\omega_c} \right] e^{-\Delta U/T}$, and that finite temperature corrections have been determined by Lifson–Jackson\(^{20}\). In the overdamped limit, Kramers' result coincides with our prediction for $\Gamma_{SD}$ obtained in our functional form for $P_c$. In the underdamped limit, $\Gamma_L$ is known to scale as $\Gamma_L \propto \frac{\Delta U}{T} \tau_{vis}^{-1} e^{-\Delta U/T}$. This result clarifies that, as concern the escape rate, the two dynamics markedly differ in the underdamped limit. The Langevin dynamics has a much higher escape rate, being $\Gamma_L/\Gamma_{SD} \propto \Delta U/T$.

**Diffusivity.** The key idea that allows to obtain analytical results for the diffusivity of a stochastically driven particle in a confining potential is the introduction of the coarse-grained trajectory illustrated in Fig. 4. Indeed, each trajectory can be conveniently described as a sequence of barrier crossing jumps, with displacement $\Delta x^0$, followed by effective intra-well jumps, with displacement $\Delta x^1$. The effective displacement $\Delta x^0$ is the total displacement of the intra-well jumps connecting the final position of jump $\Delta x^0$, and the initial position of jump...
Since the fraction of barrier-crossing jumps is $P_d$, after $Nt_N/c_j$ jumps the overall displacement is
\[
\Delta \mathbf{R}(Nt_N/c_j) = \sum_{i=1}^{N/P_d} (\Delta x_i^{\cap} + \Delta x_i^{\cup}),
\]
and the diffusion coefficient is
\[
D = \frac{1}{2t_c} \left\langle \sigma_{x_i}^2 \right\rangle = \frac{1}{2t_c} \left\langle (\Delta x_i^{\cap})^2 + (\Delta x_i^{\cup})^2 \right\rangle = D^{\cap} + D^{\cup},
\]
where $\langle \cdot \rangle$ indicates averages over uncorrelated jumps. Thus, we are left with the problem of estimating the mean square jump length of uncorrelated barrier crossing jumps, $\langle (\Delta x^{\cap})^2 \rangle$, and of uncorrelated effective intra-well jumps, $\langle (\Delta x^{\cup})^2 \rangle$.

In the overdamped $t_c \to 0$ limit all jumps are short, and barrier crossing jumps start and end close to the top of a barrier, where the potential is flat. Accordingly, $\langle (\Delta x^{\cap})^2 \rangle |_{t_c=0} \approx 12T_c^2/m^3$, and given our results for $P_d$ and $P_d$,
\[
D^{\cap}|_{t_c=0} \approx 6T_c^2P_d \approx TL^{-2}L^3 \Delta U e^{-\Delta U/T}.
\]

To estimate $\langle (\Delta x^{\cup})^2 \rangle |_{t_c=0}$, we consider that, since barrier crossing jumps are short, two subsequent barrier crossing jumps are connected by a sequence of jumps whose total displacement is either zero, if the particle recrosses the same barrier, or roughly equal to the period of the potential, if the particle traverses a well and crosses a subsequent barrier. For uncorrelated barrier crossing jumps these two possibilities are equally likely, which implies $\langle (\Delta x^{\cup})^2 \rangle |_{t_c=0} \approx L^2/2$. This allows to estimate
\[ D^{\downarrow}_{t \to 0} \approx \frac{L^2}{4} P_i \frac{P_a}{t_c} \propto \Delta U t e^{-\Delta U/T}. \]  

(6)

In the underdamped \( t_c \to \infty \) limit a particle that has enough energy to cross an energy barrier will traverse \( \Delta x^2(t, E)/L \approx t/t_{w,E} \) wells, where \( t \) is the jump duration, and \( t_{w,E} \) the time the particle needs to cross a single energy well. Thus \( \langle (\Delta x^2(t, E))^2 \rangle \approx L^2 \langle t^2 \rangle/t_{w,E} \) is evaluated averaging over the waiting time distribution \( \langle t^2 \rangle = 2t_c^2 \) and over the energy of the particle. This leads to \( \langle (\Delta x^2(t, E))^2 \rangle = 2t_c^2 L^2 \int_{-\Delta U}^{\infty} \frac{e^{-\gamma E}}{\gamma^2} dE \left( \int_{-\Delta U}^{\infty} e^{-\frac{s}{\gamma T}} \tau_{w,E} dE \right)^{-1} \), that scales as
\[ \langle (\Delta x^2) \rangle t \propto \Delta U t_c^2 \]

(7)

since \( t_{w,E} = t_f \left( \frac{L}{2} - \frac{1}{2} \right) \propto \frac{L}{\Delta U} \) for small \( E - \Delta U \). We thus estimate
\[ D^{\downarrow}_{t \to \infty} \propto \Delta U t e^{-\Delta U/T}. \]  

(8)

To determine \( \langle (\Delta x^2) \rangle t \) we indicate with \( P_i \) the probability that a walker interacts \( k \) times with the heat bath in a well, before escaping. If \( x_s \) is the original position inside the well, and \( x_f \) the final one, then \( \langle (\Delta x^2) \rangle t \propto \sum P_i \int P_s(x_f) P_r(x_i) (x_f - x_i)^2 dx_i dx_f \), where \( P_r(x_i) \) is the probability that the barrier crossing jump ends in \( x_s \), one could evaluate from the equilibrium distributions over the barrier-crossing jumps, and \( P_r(x_i) dx_i \) is the probability that the jump through which the particle escapes from the well starts in \( x_s \), being the particle arrived in \( x_s \). To a good approximation a particle exits from the well after performing a single collision, so that \( x_f - x_i = 0 \), or after thermalizing within the well, so that \( x_s \) and \( x_e \) become uncorrelated. Accordingly,
\[ \langle (\Delta x^2) \rangle t \propto P_i \cdot 0 + (1 - P_i) \langle \lambda^2 \rangle, \]

where
\[ \langle \lambda^2 \rangle t \propto \int_{-L/2}^{L/2} P_s(x_e, T) P_r(x_i, T)(x_f - x_i)^2 dx_i dx_f, \]

(9)

with \( P_r(x_f, T) \) the probability that a barrier crossing jumps of a thermalized state starts from position \( x_i \). The evaluation of both \( P_i, P_r(x_i, T) \) and \( P_r(x_i, T) \) leads to \( \langle (\Delta x^2) \rangle t \propto L^2 \). Summarizing, in the \( t \to \infty \) limit
\[ D^{\downarrow}_{t \to \infty} = \frac{P_i}{2t_c} \langle (\Delta x^2) \rangle t \propto \frac{L^2}{t_c} \exp(-\Delta U/T). \]

(10)

We finally note that, in both Eqs 8 and 10, the proportionality constants have a weak temperature dependence we neglect, that is fixed by the shape of the potential.

While we have estimated \( D^{\downarrow}_{t \to \infty} \) and \( D^{\downarrow}_{t \to \infty} \) in the low temperature regime, it is also possible to estimate \( D^{\downarrow}(t_c) \) at all \( t \). To this end we assume the barrier crossing jumps to be always uncorrelated, which is reasonable as the jumps are uncorrelated both in the overdamped limit, as jumps are short and particles on the top of the barrier as well as in the underdamped limit. With this assumption we estimate \( \langle (\Delta x^2) \rangle t \) from equilibrium average over the jumps, \( \langle (\Delta x^2) \rangle t \propto \int_{-L/2}^{L/2} dx_i \int_{-L/2}^{L/2} dx_f \int_{-\Delta U}^{\infty} dx_i \int_{-\Delta U}^{\infty} dx_f \exp(-\gamma E/2T) \), with \( f \) given in Eq. 2, and thus get \( D^{\downarrow}(t_c) = \frac{1}{2} t_c^2 P_i \langle (\Delta x^2) \rangle t \). Beside being valid at all \( t \), in the low temperature regime, this prediction is also valid at all temperatures in the underdamped regime, where \( P_i = 1 \). Figure 5 illustrates that this theoretical prediction (dashed line) correctly describes the numerical data (full circles), and scales as \( t_c^2 \) in the overdamped and in the underdamped limit, as predicted in Eqs 5 and 8, respectively. In the figure, we also illustrate numerical results for the contribution to the diffusion coefficient of the intra-well jumps (full diamonds), that behaves as predicted in Eqs 6 and 10 in two limits. Thus, the overall diffusion coefficient exhibits a crossover between two linear regimes, as \( D \approx D^{\downarrow} \) in the overdamped limit, and \( D \approx D^{\downarrow} \) in the underdamped one.

We finally compare the diffusion coefficient of the Stochastically Driven and of the Langevin dynamics, identifying their characteristic timescales, \( \tau = t_c = t_{w,E} \). For both dynamics \( D = \Gamma / \Delta U \) in the overdamped limit. In this limit, the full van Hove distributions actually coincide at all times. In the underdamped low temperature limit, the diffusivity of the Langevin dynamics is \( D_{\Gamma, SD} \propto \Delta U / (T \tau) \), while that of the Stochastically Driven particle is given by Eq. 8, \( D \propto \Delta U t e^{-\Delta U/T} \). Accordingly, in this limit the Stochastically Driven dynamics is faster than the Langevin one, as illustrated in Fig. 6a. Figure 6b compares the diffusivities of the two dynamics as concern their temperature dependence, in the underdamped regime. The numerical results for the temperature dependence of the Stochastically Driven particle diffusivity are correctly described by our theoretical prediction for \( D^{\downarrow} \) valid at all temperatures (full line), while those of the Langevin dynamics have been predicted in ref. 22. At high temperature, \( T > \Delta U \), the effect of the potential is negligible and the two diffusivities coincide, and scale as \( T^2 e^{-2\Delta U/T} / \Delta U \). In the low temperature regime, the Langevin diffusivity does not change temperature dependence, while the diffusivity of the Stochastically Driven particle model only depends on temperature through the Arrhenius factor. The difference in the diffusivities in the underdamped low temperature regime is rationalized considering that the two dynamics are mapped on free hopping dynamics with a different jump rate \( \Gamma \), and a different mean square jump length, \( \lambda^2 \). Indeed, on the one side we have already seen that \( \Gamma / \Gamma_{SD} \propto \Delta U / T \). On the other side, in the underdamped limit the mean square size of the jumps of the Langevin dynamics as \( \langle \lambda^2 \rangle_{SD} \propto T^2 e^{-2\Delta U/T} / \Delta U \), while that of the Stochastically Driven dynamics scales as \( \langle \lambda^2 \rangle_{SD} \propto \Delta U t_c^2 \), as in Eq. 7, so that \( \langle \lambda^2 \rangle / \langle \lambda^2 \rangle_{SD} \propto (T / \Delta U)^2 \).
Thus, despite making more frequent irreversible barrier crossing jumps, the Langevin dynamics has a smaller diffusivity as its jumps are much shorter.

**Discussion**

We put forward an analytical treatment of the escape rate from a well and of the diffusion coefficient in a periodic potential of a Stochastically Driven particle, considering both the overdamped and the underdamped limits. The particle behaves as a Langevin particle in the overdamped limit. In the underdamped low temperature limit, conversely, with respect to a Langevin particle a Stochastically Driven one has a smaller escape rate, but a larger diffusion coefficient.
Our observations are relevant to describe the dynamics of systems that undergo infrequent collisions with bath particles. Thus, our results could describe chemical reactions occurring at very low pressure, as in this case gas particles seldom collide with the system of interest. Similarly, our results could be relevant to discuss diffusion in amorphous materials at low temperature, when the system can be seen as hopping through different minima of its energy landscape. In this case, the heat bath is provided by the scattering of phonons, whose collision frequency is small at low temperatures.

An interesting feature of this model, which is also observed in a variety of soft-matter and biological systems, is the long coexistence of a van Hove distribution with non-gaussian tails, and of a mean square displacement linear in time. An important open question ahead concerns the temporal evolution of the van Hove distribution in the underdamped limit, to rationalize how normal diffusion is recovered.

### Methods

**Simulation details.** In the Stochastically Driven dynamics, a particle in position \( x_t = x(t) \) that collides with the heat bath acquires a velocity \( v = v(t) \) and an energy \( E = V(x) + mv^2/2 \). This energy is conserved up to the time \( t_c = t + \Delta t \) of the next collision of the particle with the heat bath. At time \( t_c \), the particle will be in position \( x_c \), the end-point of the jump. In the overdamped and intermediate regime we determine \( x_c \) by numerically integrating the equation of motion during a jump, i.e. from the time of the collision \( t_t \) to the time \( t_c \), using a simple explicit Euler scheme. In the underdamped regime, it is computationally convenient to follow a different approach. Suppose, for instance, that after a collision a particle has enough energy to overcome an energy barrier. In this case the particle will actually traverse many wells, as the jump duration \( \Delta t \) is large. Let \( \Delta t_{\text{hop}} \) the time the particle needs to reach the top of the barrier, and \( \Delta t_{\text{cross}} \) the time it needs to traverse a well. Starting, without loss of generality, from the first well with positive velocity, the arrival point is conveniently estimated as \( x_c = x_t + (L/2 - x_t) + ln + \Delta x, \) where \( n \) is the integer part of \( (\Delta t - \Delta t_{\text{hop}})/\Delta t_{\text{cross}} \) and \( \Delta x \) is the distance the particle moves from the top in a time \( \Delta t - \Delta t_{\text{hop}} - n \Delta t_{\text{cross}} \). This expression for \( x_c \) is convenient as the various quantities can be analytically computed, for our model potential. However, their evaluation requires the evaluation of an elliptic integral, which is time consuming. Thus, this approach is actually convenient only in the underdamped regime. A similar approach can be used when the particle has not enough energy to cross an energy barrier, in which case the particle will perform many oscillations within a well, in the underdamped regime.

The simulation of the Langevin dynamics is more time-consuming that that of the Stochastically Driven dynamics. We have carried it out fixing the integration timestep at \( 10^{-2} \omega_b t_c \).

**Measurement of \( P_{\gamma} \) and \( P_{d} \).** \( P_{\gamma} \) the probability that a jump crosses a barrier, is easily determined in simulations as the long time limit of the ratio between the number of barrier crossing jumps, \( M(t) \), and the total number of jumps, \( N(t) \): \( P_{\gamma} = \lim_{t \to \infty} M(t)/N(t) \). This is the quantity represented by the data points of Fig. 2a. \( P_d \) is the fraction of barrier crossing jumps that are irreversible, i.e. which are followed with equal probability by a forward or by a backward jump. Operatively, this quantity is measured in the simulation by recording the number of forward jumps \( f(t) \), which are the jumps having the same direction of their predecessor, and the number of backwards jumps, \( b(t) \). Thus, the total number of barrier crossing jumps is \( M(t) = f(t) + b(t) \), and \( P_d = \lim_{t \to \infty} 2f(t)/M(t) \).

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M.P.C. and A.P. conceived the project, A.P. carried out simulations, M.P.C. and A.P. wrote the paper.

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