

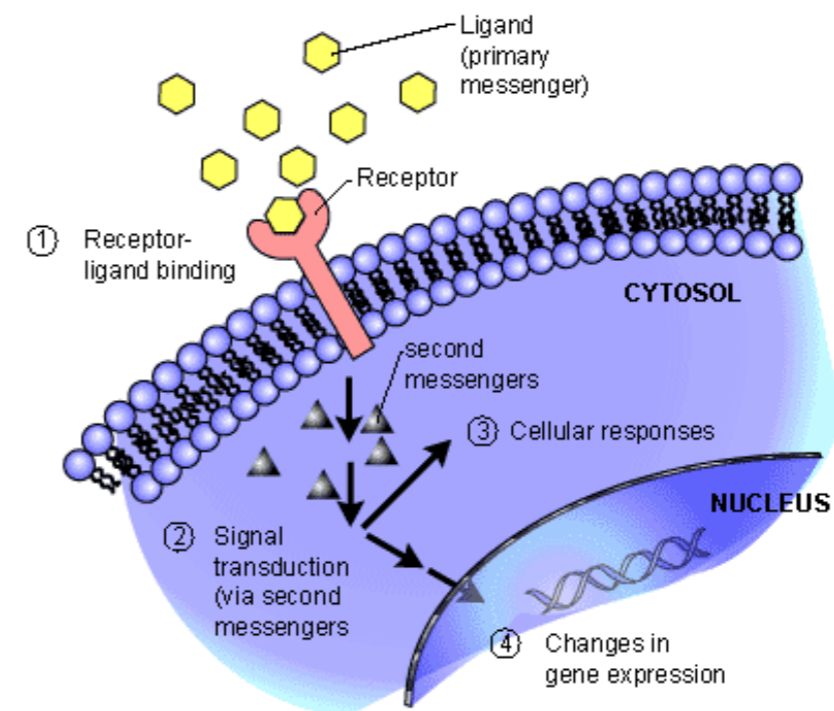
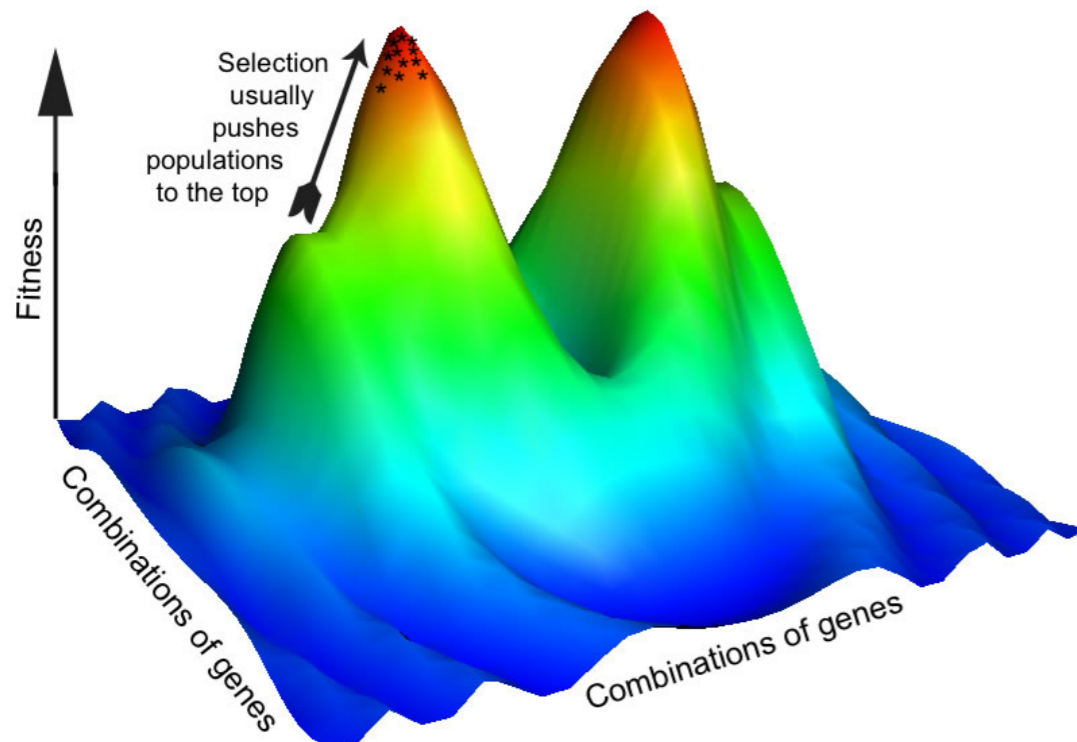
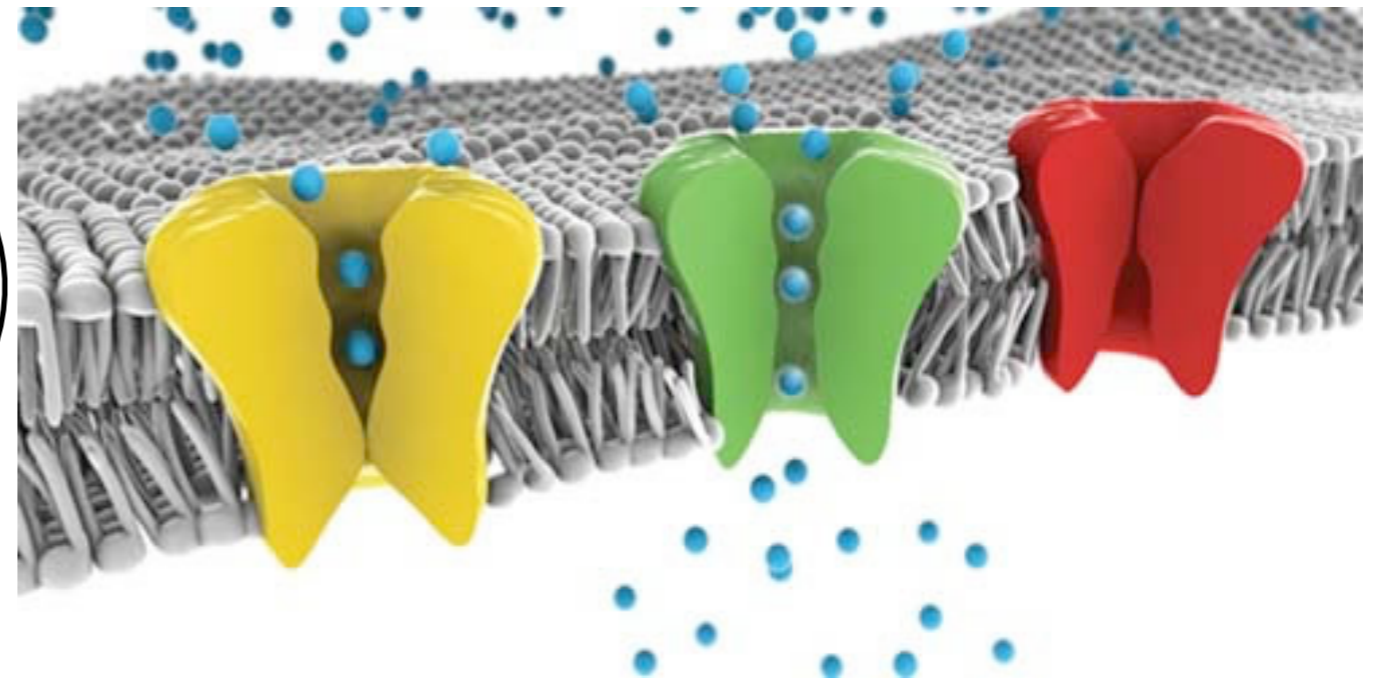
Escape Problems & Stochastic Resonance

18.S995 - L08 & 09

Examples

transport & evolution:
stochastic
escape problems

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Reaction-rate theory: fifty years after Kramers

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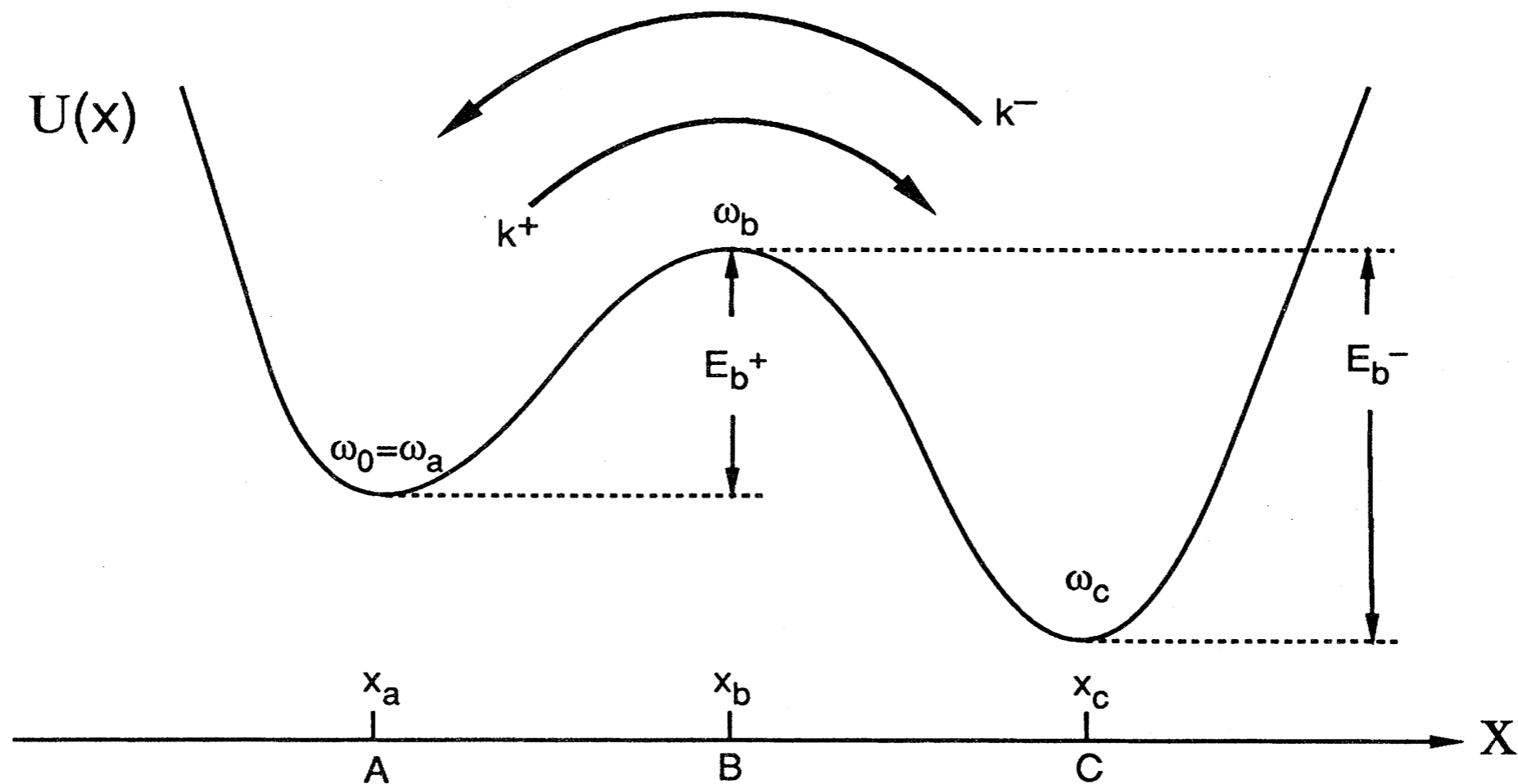


FIG. 3. Potential $U(x)$ with two metastable states A and C . Escape occurs via the forward rate k^+ and the backward rate k^- , respectively, and E_b^\pm are the corresponding activation energies.

Arrhenius law

$$k = \nu \exp(-\beta E_b)$$

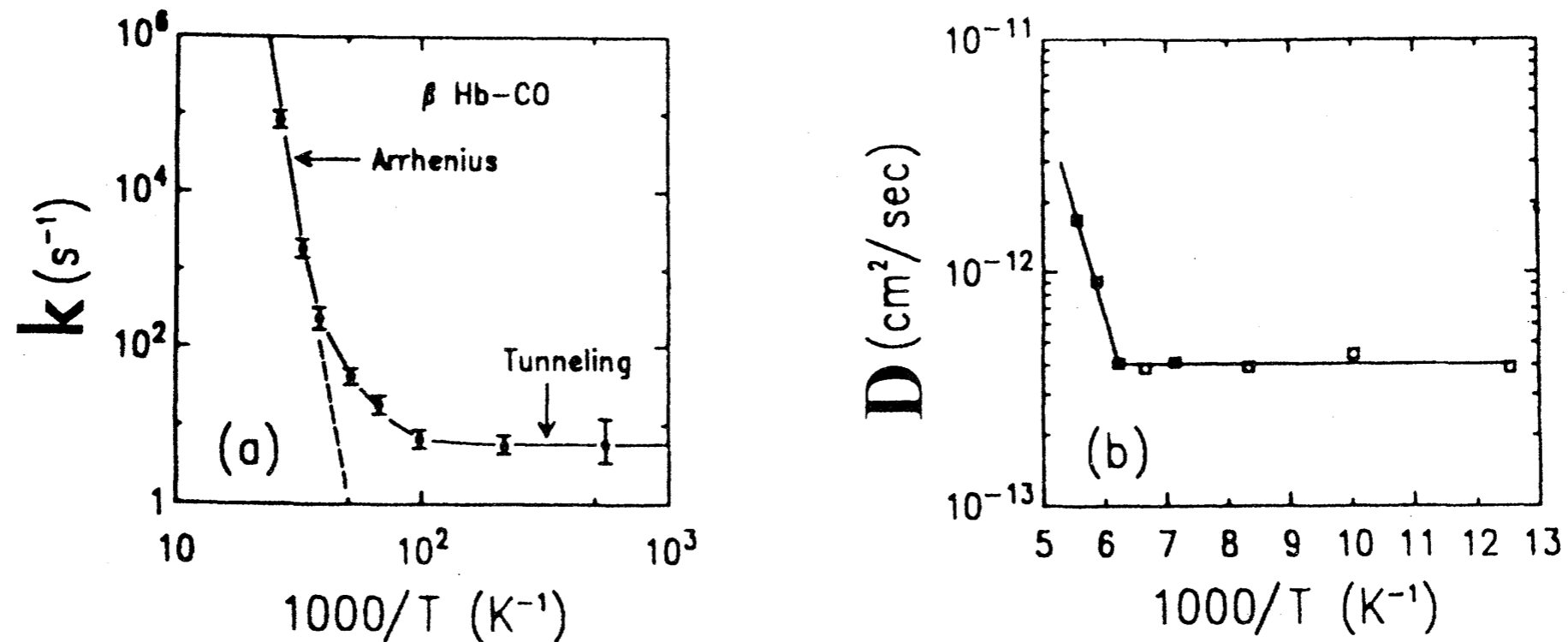
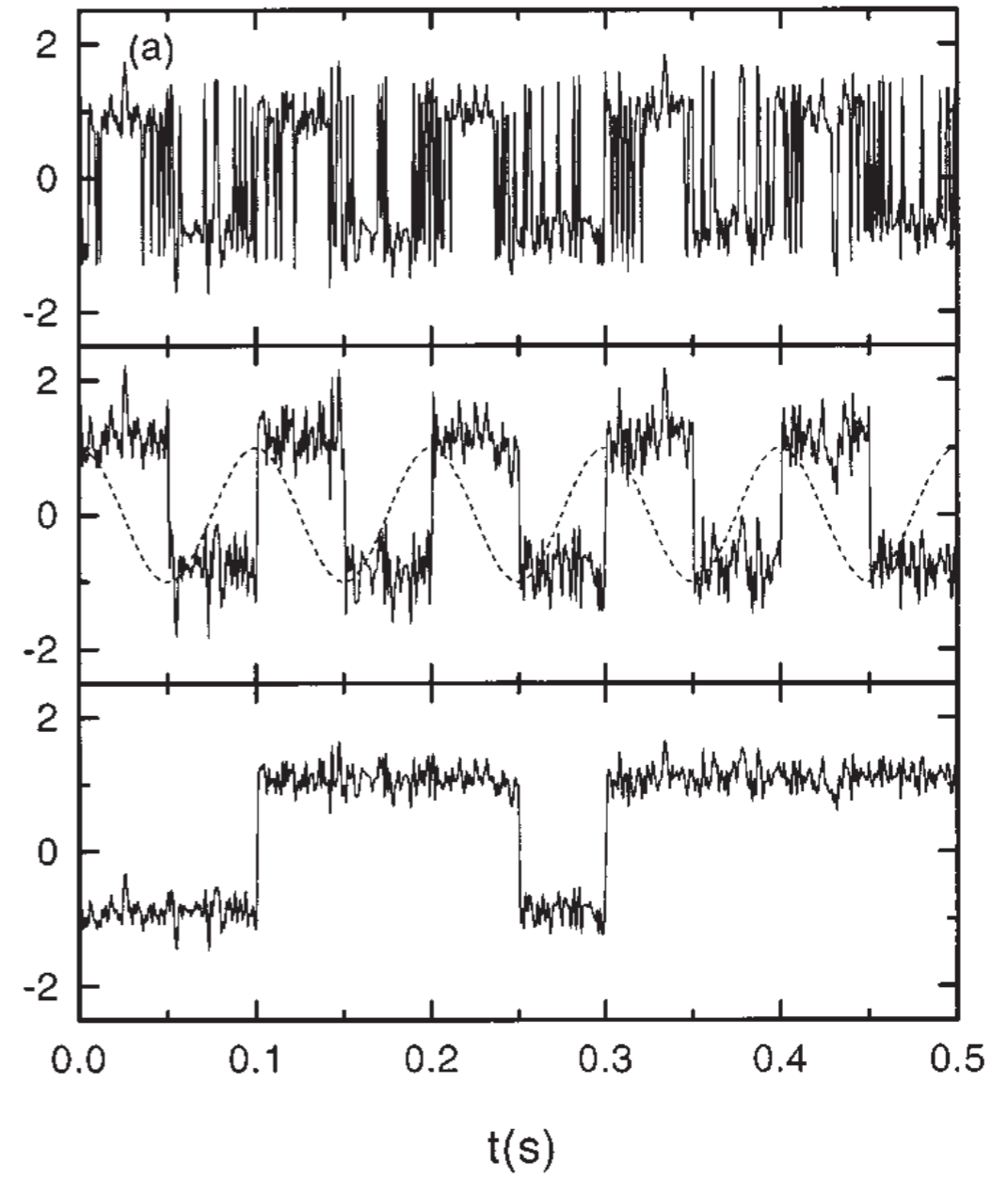
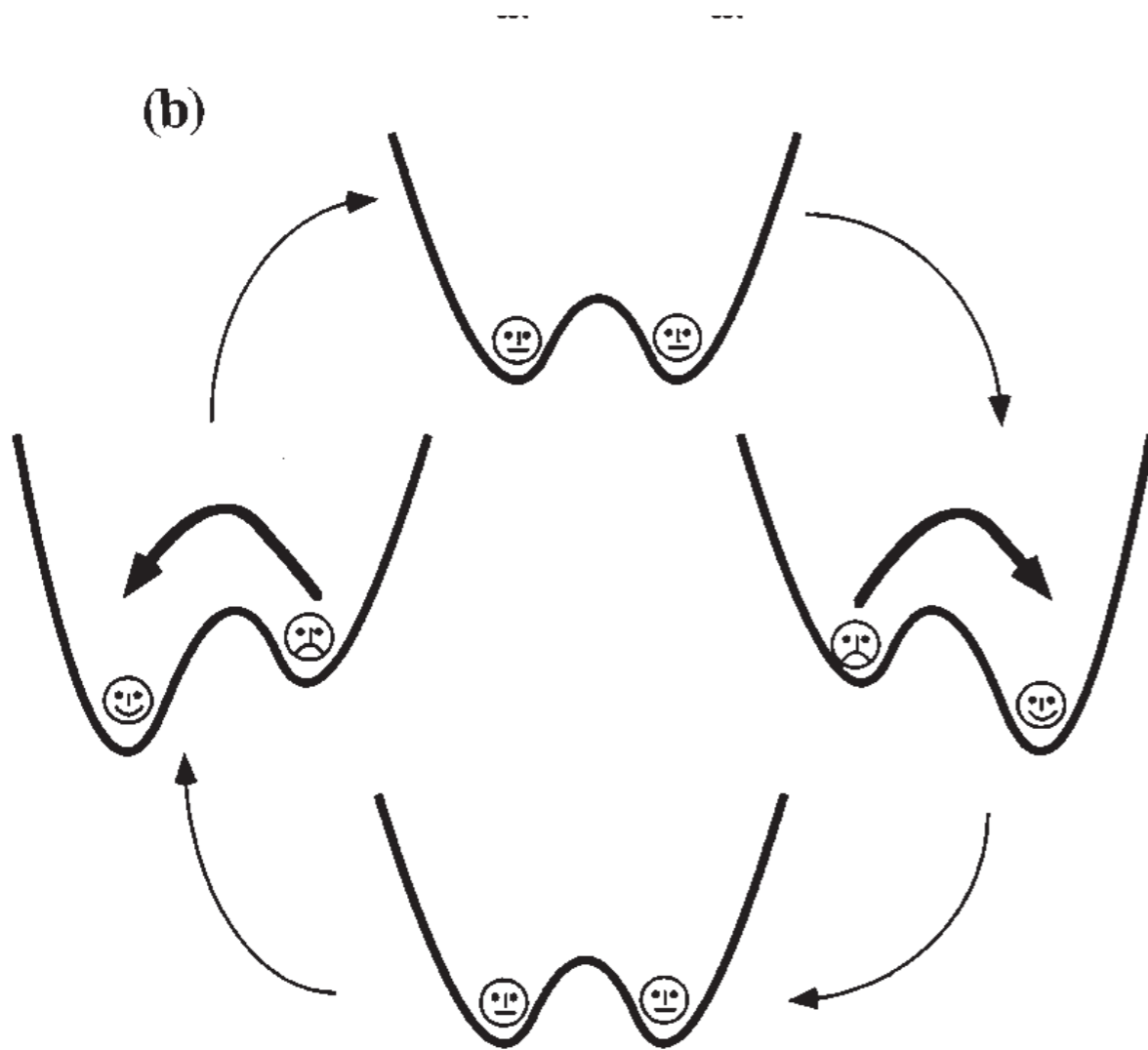


FIG. 2. Van't Hoff-Arrhenius plots of reaction-rate data for two different physical systems in which both thermal activation and tunneling events occur: (a) Rate of CO migration to a separated β chain of hemoglobin (Alberding *et al.*, 1976; Frauenfelder, 1979); (b) diffusion coefficient D of atomic hydrogen moving on the (110) plane of tungsten at a relative H -coverage of 0.1 (data taken from DiFoggio and Gomer, 1982). The diffusion D is directly proportional to the hopping rate k .

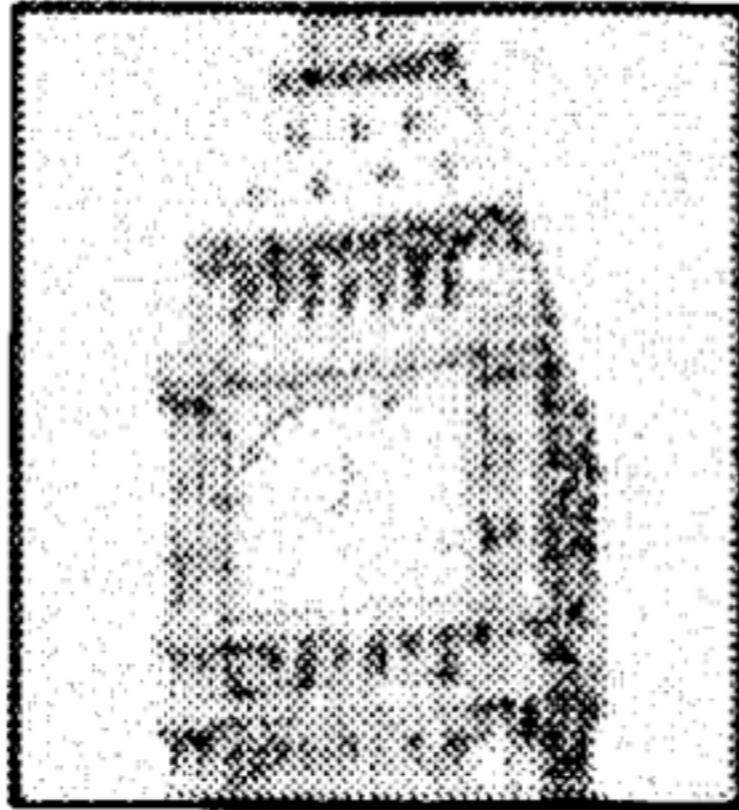
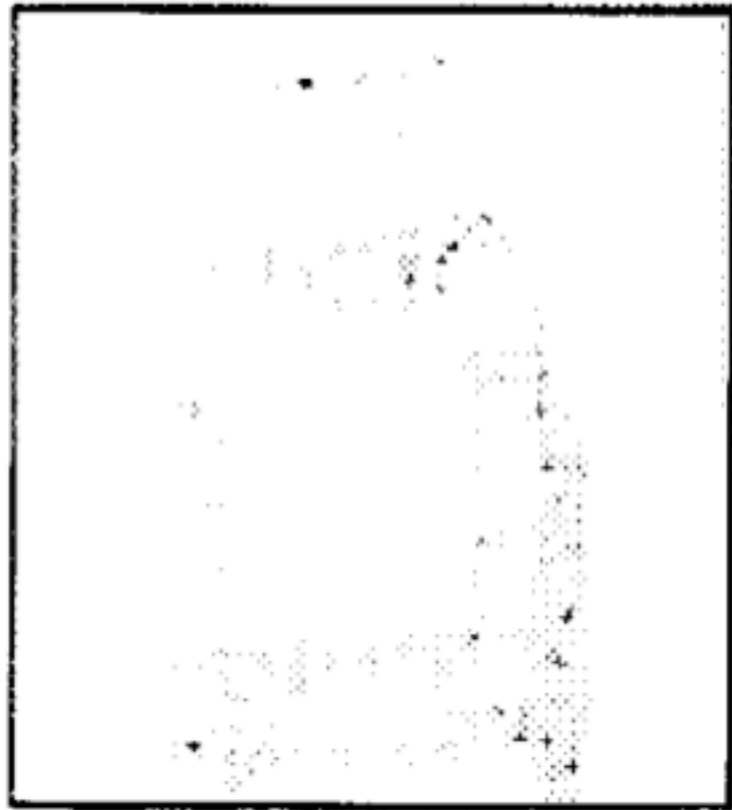
Stochastic resonance

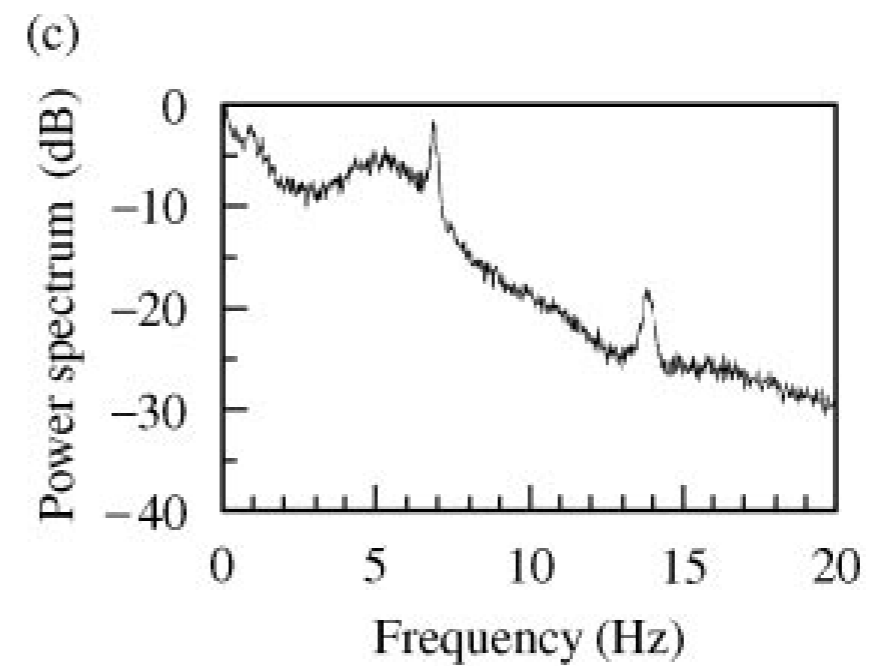
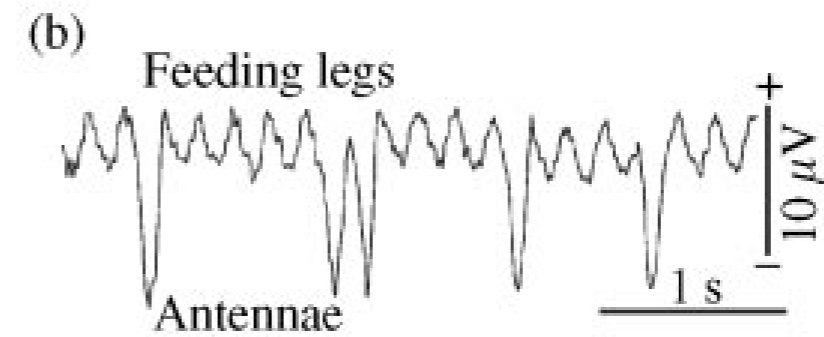
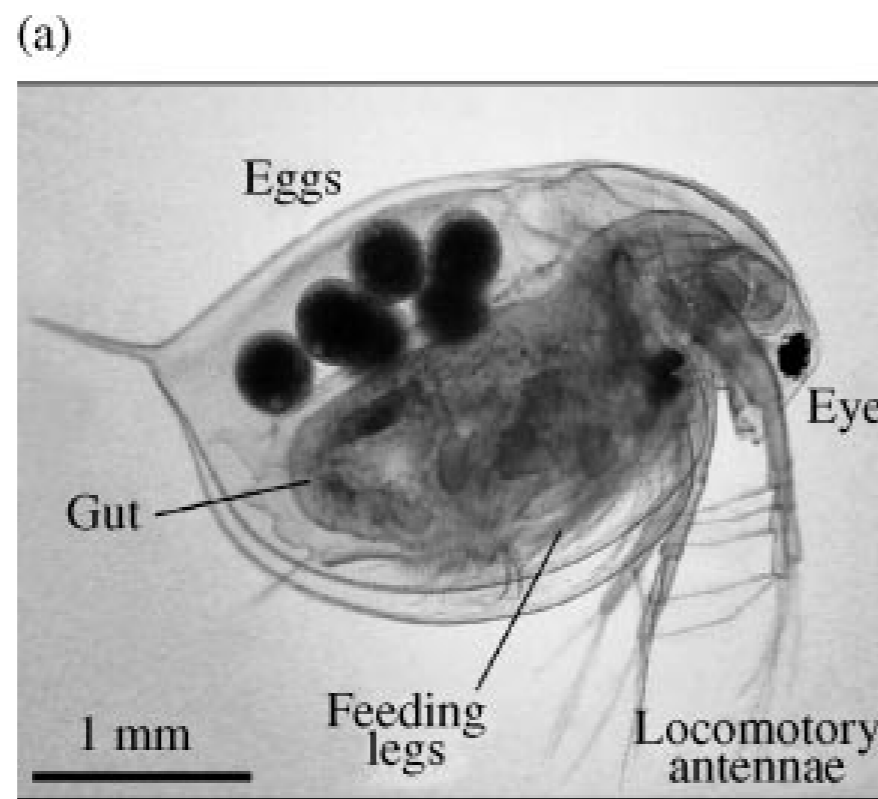
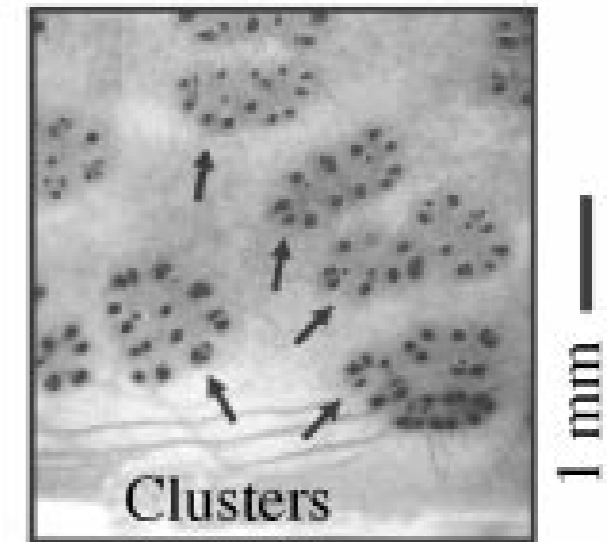
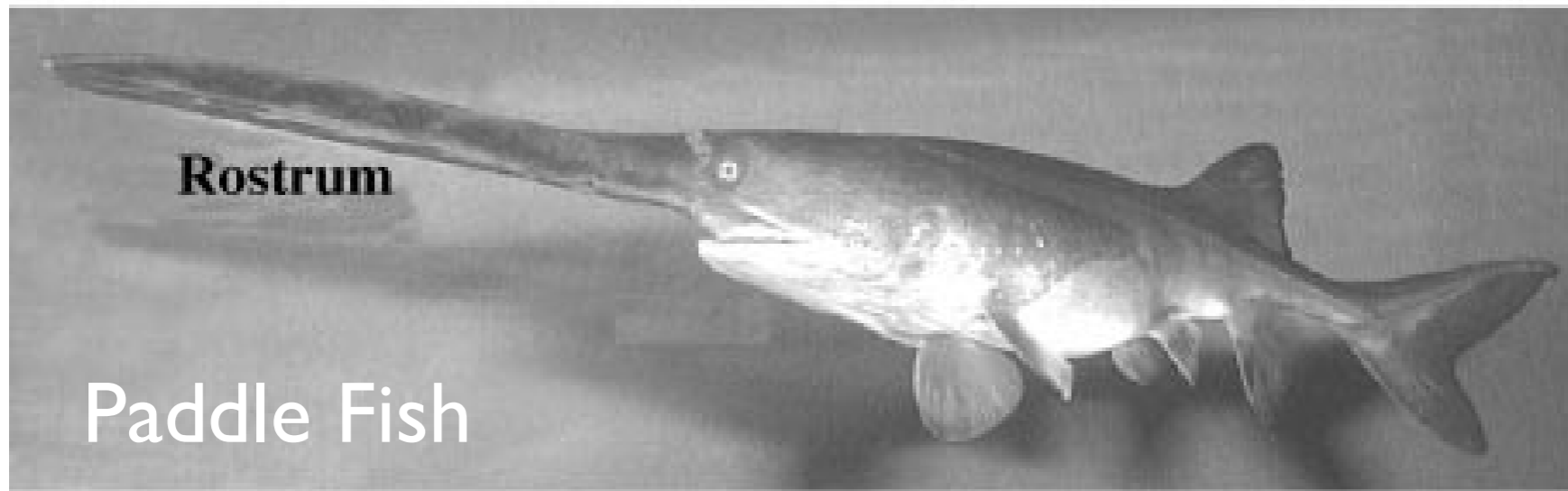


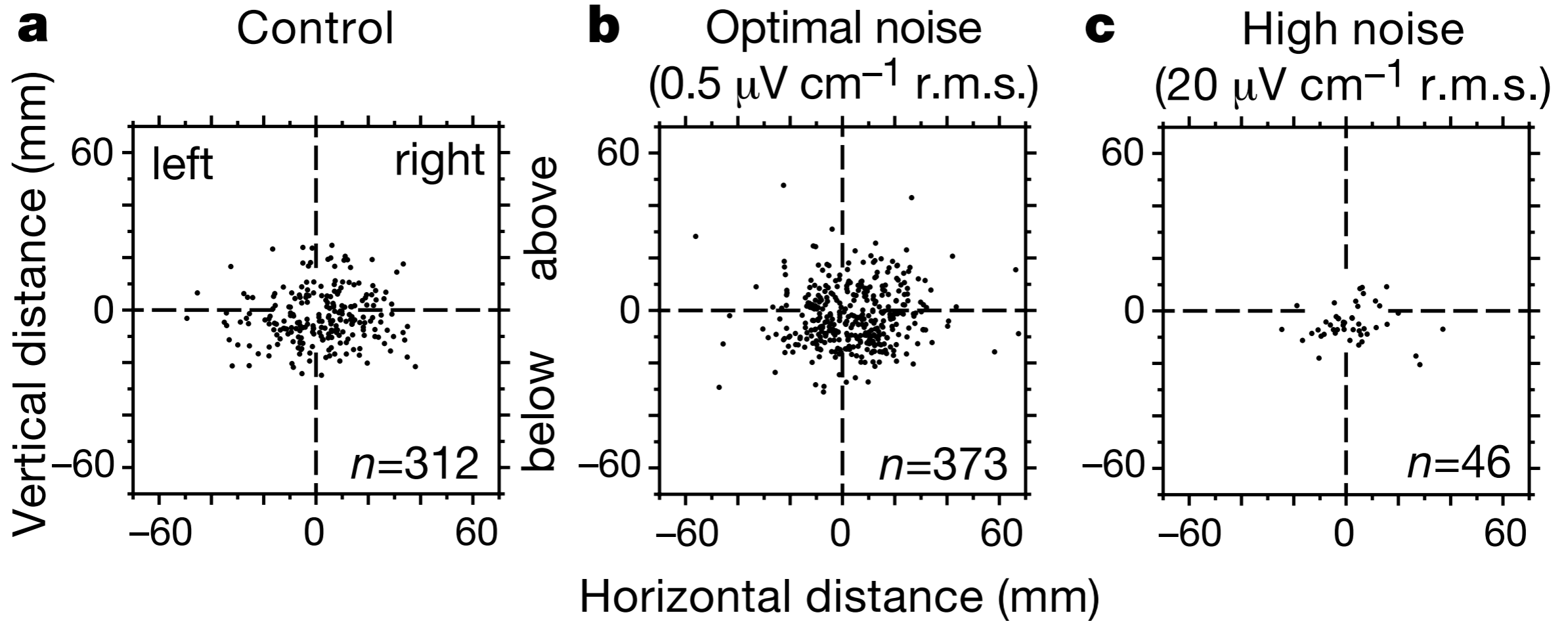
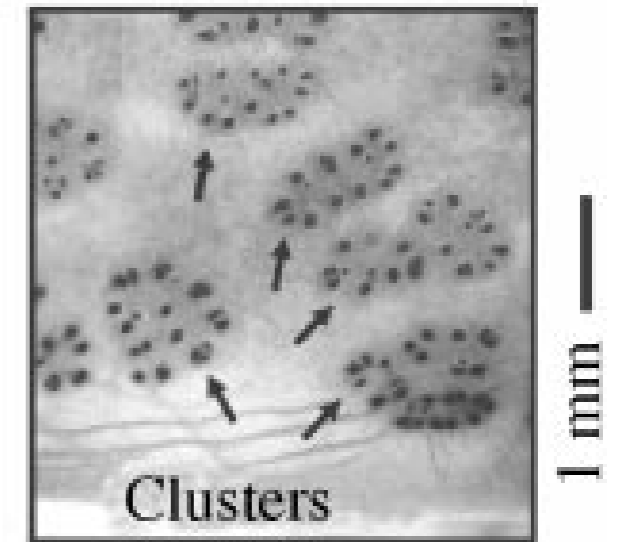
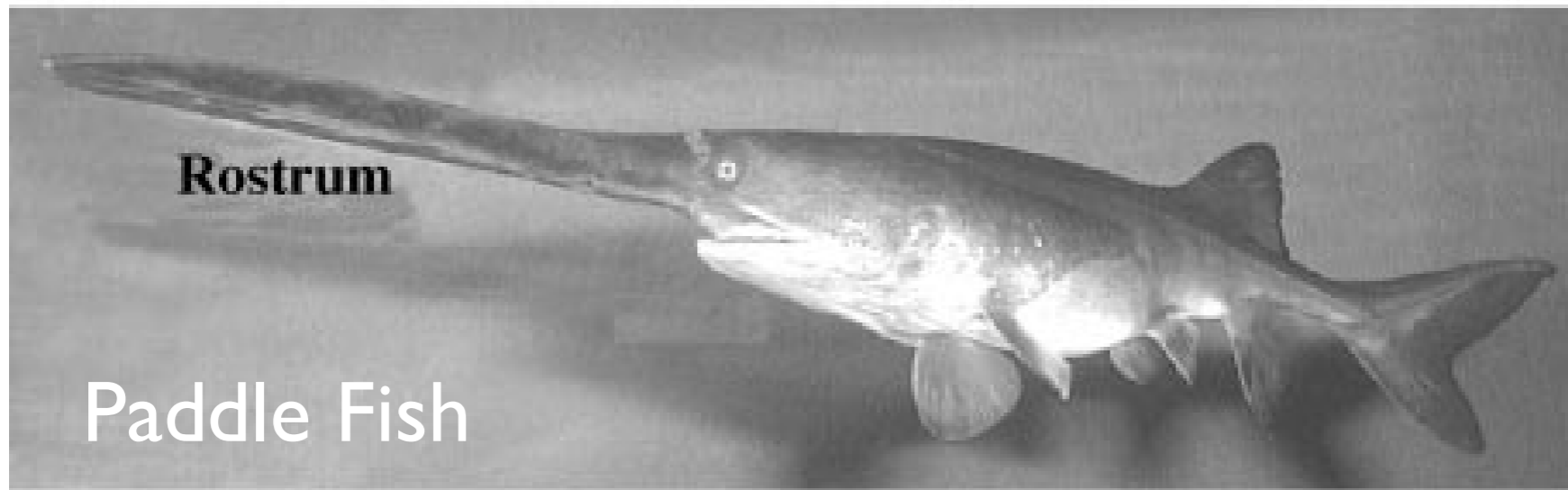
Using **fitness landscapes** to visualize **evolution in action**

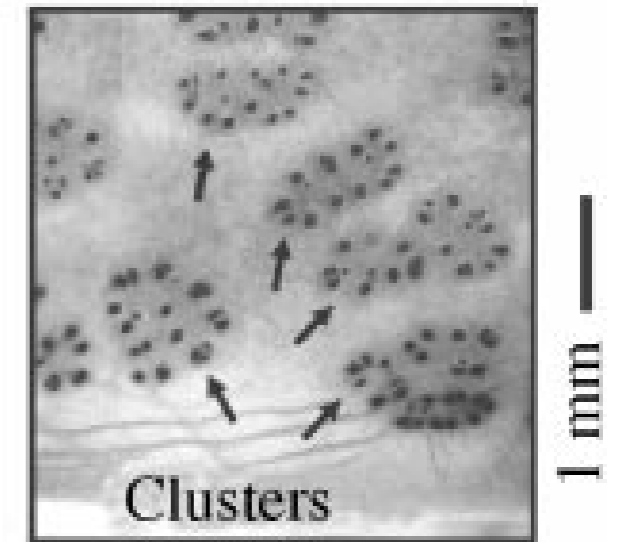
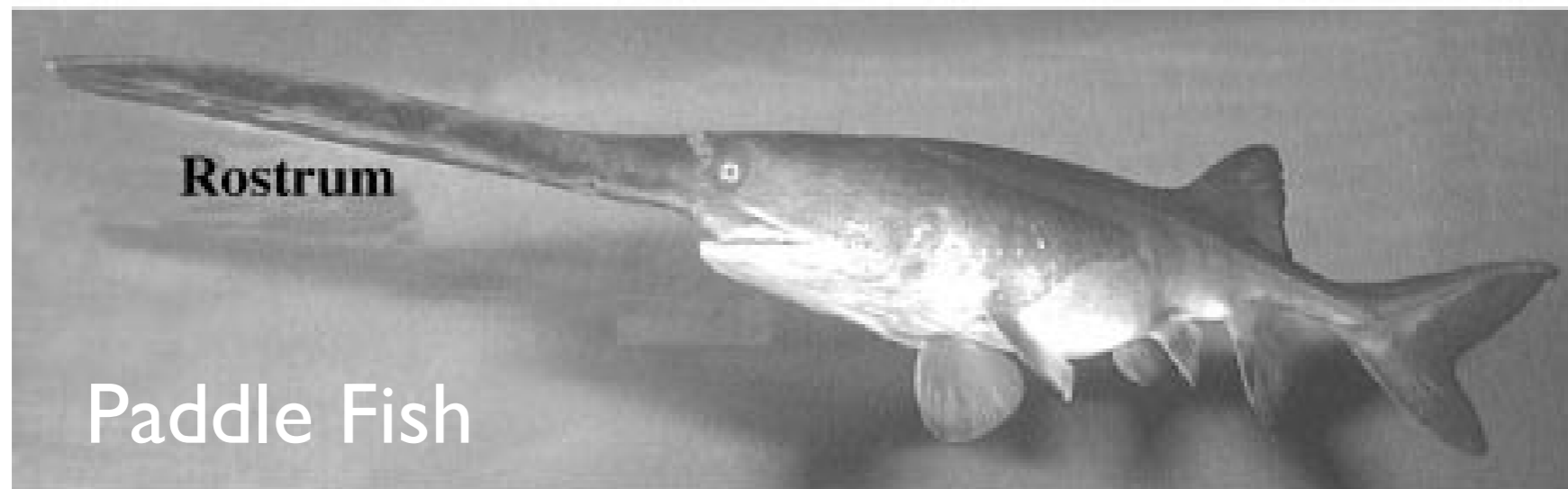
A film by Randy Olson and Bjørn Østman

<https://www.youtube.com/watch?v=4pdiAneMMhU>









sensory system. However, stochastic resonance requires an external source of electrical noise in order to function. A swarm of plankton, for example *Daphnia*, can provide the required noise. We hypothesize that juvenile paddlefish can detect and attack single *Daphnia* as outliers in the vicinity of the swarm by using noise from the swarm itself. From the power spectral density of the noise plus the weak signal from a single *Daphnia*, we calculate the signal-to-noise ratio, Fisher information and discriminability at the surface of the paddlefish's rostrum. The results predict a specific attack pattern for the paddlefish that appears to be experimentally testable.

1.4.1 Generic minimal model

Consider the over-damped SDE

$$dx(t) = -\partial_x U dt + \sqrt{2D} * dB(t) \quad (1.68a)$$

with a confining potential $U(x)$

$$\lim_{x \rightarrow \pm\infty} U(x) \rightarrow \infty \quad (1.68b)$$

that has two (or more) minima and maxima. A typical example is the bistable quartile double-well

$$U(x) = -\frac{a}{2}x^2 + \frac{b}{4}x^4, \quad a, b > 0 \quad (1.68c)$$

with minima at $\pm\sqrt{a/b}$.

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Generally, we are interested in characterizing the transitions between neighboring minima in terms of a rate k (units of time^{-1}) or, equivalently, by the typical time required for escaping from one of the minima. To this end, we shall first discuss the general structure of the time-dependent solution of the FPE¹⁴ for the corresponding PDF $p(t, x)$, which reads

$$\partial_t p = -\partial_x j, \quad j(t, x) = -[(\partial_x U)p + D\partial_x p], \quad (1.68d)$$

and has the stationary zero-current ($j \equiv 0$) solution

$$p_s(x) = \frac{e^{-U(x)/D}}{Z}, \quad Z = \int_{-\infty}^{+\infty} dx e^{-U(x)/D}. \quad (1.69)$$

General time-dependent solution

$$\partial_t p = -\partial_x j, \quad j(t, x) = -[(\partial_x U)p + D\partial_x p], \quad (1.68d)$$

To find the time-dependent solution, we can make the ansatz

$$p(t, x) = \varrho(t, x) e^{-U(x)/(2D)}, \quad (1.70)$$

which leads to a Schrödinger equation in imaginary time

$$-\partial_t \varrho = [-D\partial_x^2 + W(x)] \varrho =: \mathcal{H}\varrho, \quad (1.71a)$$

with an effective potential

$$W(x) = \frac{1}{4D}(\partial_x U)^2 - \frac{1}{2}\partial_x^2 U. \quad (1.71b)$$

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Assuming the Hamilton operator \mathcal{H} has a discrete non-degenerate spectrum, $\lambda_0 < \lambda_1 < \dots$, the general solution $p(t, x)$ may be written as

$$p(t, x) = e^{-U(x)/(2D)} \sum_{n=0}^{\infty} c_n \phi_n(x) e^{-\lambda_n t}, \quad (1.72a)$$

where the eigenfunctions ϕ_n of \mathcal{H} satisfy

$$\int dx \phi_n^*(x) \phi_m(x) = \delta_{nm}, \quad (1.72b)$$

and the constants c_n are determined by the initial conditions

$$c_n = \int dx \phi_n^*(x) e^{U(x)/(2D)} p(0, x). \quad (1.72c)$$

General time-dependent solution

$$p(t, x) = e^{-U(x)/(2D)} \sum_{n=0}^{\infty} c_n \phi_n(x) e^{-\lambda_n t}$$

At large times, $t \rightarrow \infty$, the solution (1.72a) must approach the stationary solution (1.69), implying that

$$\lambda_0 = 0, \quad c_0 = \frac{1}{\sqrt{Z}}, \quad \phi_0(x) = \frac{e^{-U(x)/(2D)}}{\sqrt{Z}}. \quad (1.73)$$

Note that $\lambda_0 = 0$ in particular means that the first non-zero eigenvalue $\lambda_1 > 0$ dominates the relaxation dynamics at large times and, therefore,

$$\tau_* = 1/\lambda_1 \quad (1.74)$$

is a natural measure of the escape time. In practice, the eigenvalue λ_1 can be computed by various standard methods (WKB approximation, Ritz method, techniques exploiting supersymmetry, etc.) depending on the specifics of the effective potential W .

1.4.2 Two-state approximation

We next illustrate a commonly used simplified description of escape problems, which can be related to (1.74). As a specific example, we can again consider the escape of a particle from the left well of a symmetric quartic double well-potential

$$U(x) = -\frac{a}{2}x^2 + \frac{b}{4}x^4, \quad p(0, x) = \delta(x - x_-) \quad (1.75a)$$

where

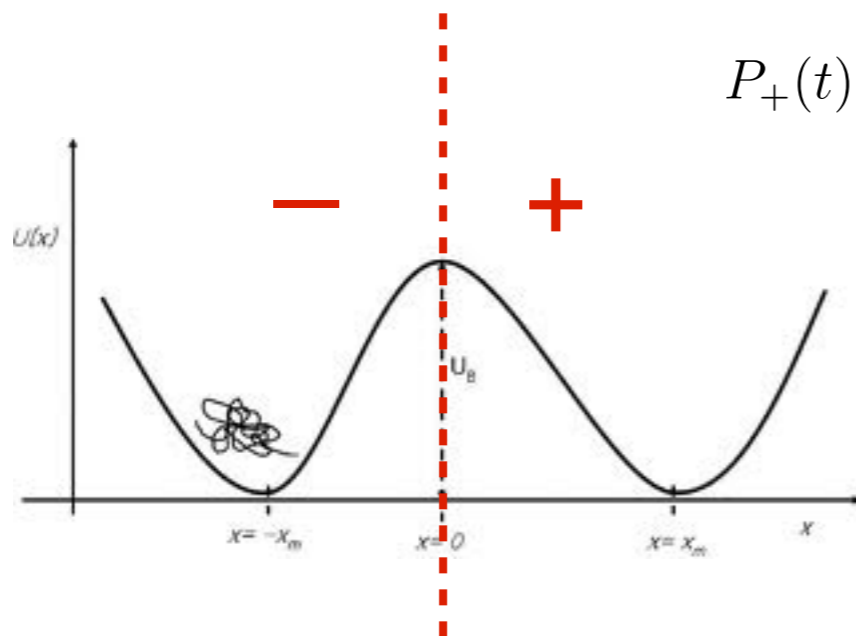
$$x_- = -\sqrt{a/b} \quad (1.75b)$$

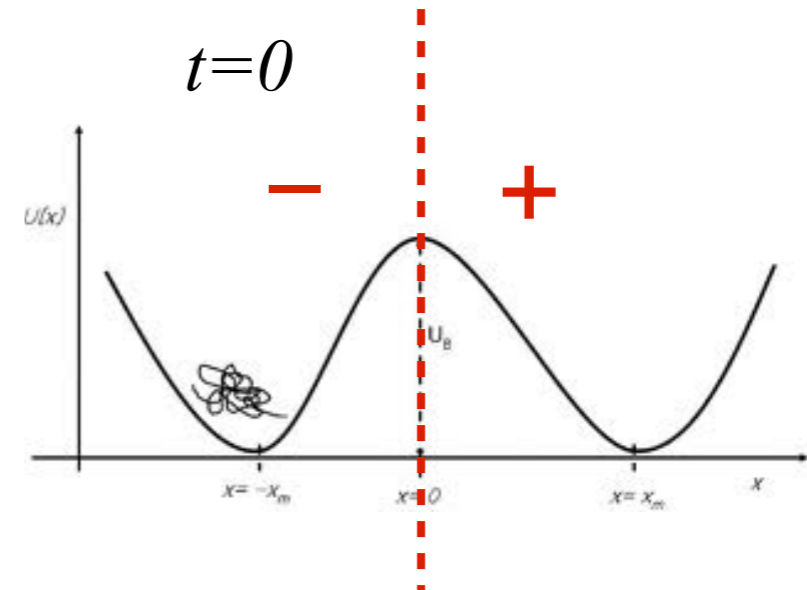
is the location of the left minimum, but the general approach is applicable to other types of potentials as well.

The basic idea of the two-state approximation is to project the full FPE dynamics onto simpler set of master equations by considering the probabilities $P_{\pm}(t)$ of the coarse-grained particle-states ‘left well’ (−) and ‘right well’ (+), defined by

$$P_-(t) = \int_{-\infty}^0 dx p(t, x), \quad (1.76a)$$

$$P_+(t) = \int_0^{\infty} dx p(t, x). \quad (1.76b)$$





If all particles start in the left well, then

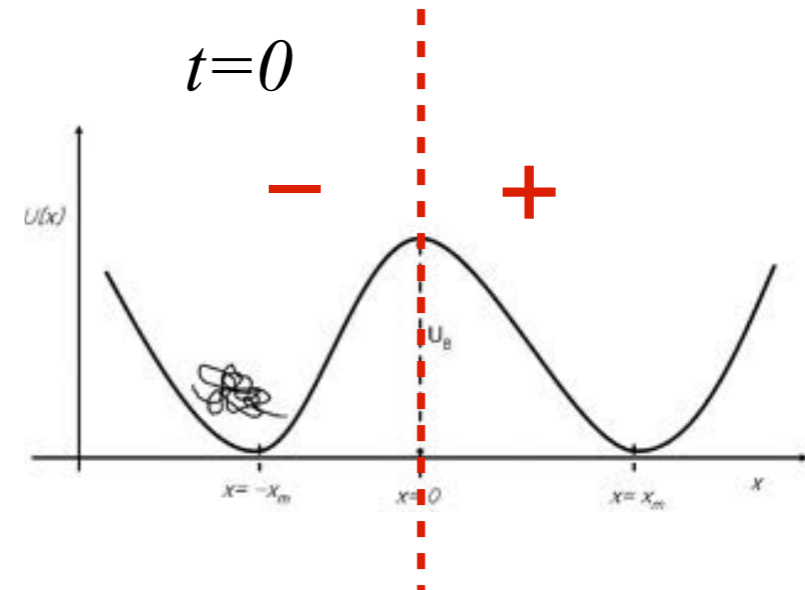
$$P_-(0) = 1, \quad P_+(0) = 0. \quad (1.77)$$

Whilst the exact dynamics of $P_{\pm}(t)$ is governed by the FPE (1.68d), the two-state approximation assumes that this dynamics can be approximated by the set of master equations¹⁵

$$\dot{P}_- = -k_+ P_- + k_- P_+, \quad \dot{P}_+ = k_+ P_- - k_- P_+. \quad (1.78)$$

For a symmetric potential, $U(x) = U(-x)$, forward and backward rates are equal, $k_+ = k_- = k$, and in this case, the solution of Eq. (1.78) is given by

$$P_{\pm}(t) = \frac{1}{2} \mp \frac{1}{2} e^{-2kt}. \quad (1.79)$$



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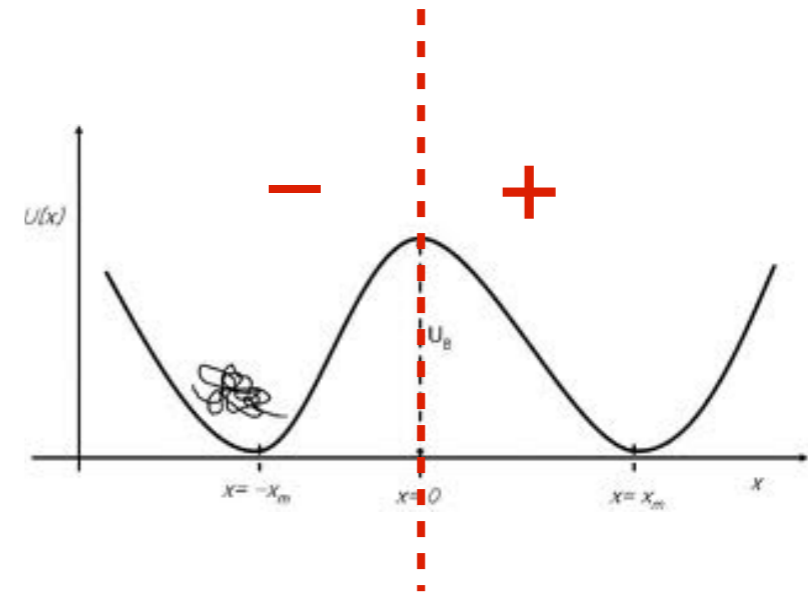
For comparison, from the FPE solution (1.72a), we find in the long-time limit

$$p(t, x) \simeq p_s(x) + c_1 e^{-U(x)/2D} \phi_1(x) e^{-\lambda_1 t}, \quad (1.80)$$

Due to the symmetry of $p_s(x)$, we then have

$$P_-(t) \simeq \frac{1}{2} + C_1 e^{-\lambda_1 t} \quad (1.81a)$$

¹⁵Note that Eqs. (1.78) conserve the total probability, $P_-(t) + P_+(t) = 1$.



Solution

$$P_-(t) \simeq \frac{1}{2} + C_1 e^{-\lambda_1 t}$$

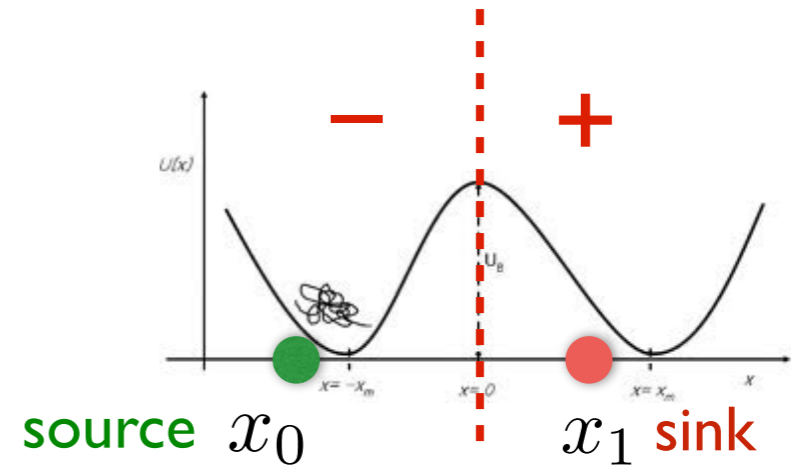
where

$$C_1 = c_1 \int_{-\infty}^0 e^{-U(x)/2D} \phi_1(x) \, dx, \quad c_1 = \phi_1^*(x_-) e^{U(x_-)/(2D)}. \quad (1.81b)$$

Since Eq. (1.81a) neglects higher-order eigenfunctions, C_1 is in general not exactly equal but usually close to $1/2$. But, by comparing the time-dependence of (1.81a) and (1.79), it is natural to identify

$$k \simeq \frac{\lambda_1}{2} = \frac{1}{2\tau_*}. \quad (1.82)$$

We next discuss, by considering in a slightly different setting, how one can obtain an explicit result for the rate k in terms of the parameters of the potential U .



1.4.3 Constant-current solution

Consider a bistable potential as in Eq. (1.75), but now with a particle source at $x_0 < x_- < 0$ and a sink¹⁶ at $x_1 > x_b = 0$. Assuming that particles are injected at x_0 at constant flux $j(t, x) \equiv J = \text{const}$, the escape rate can be defined by

$$k := \frac{J}{P_-}, \quad (1.83)$$

with P_- denoting the probability of being in the left well, as defined in Eq. (1.76a) above. To compute the rate from Eq. (1.83), we need to find a stationary constant flux solution $p_J(x)$ of Eq. (1.68d), satisfying $p_J(x_1) = 0$ and

$$J = -(\partial_x U)p_J - D\partial_x p_J \quad (1.84)$$

for some constant J . This solution is given by [HTB90]

$$p_J(x) = \frac{J}{D} e^{-U(x)/D} \int_x^{x_1} dy e^{U(y)/D}, \quad (1.85)$$

as one can verify by differentiation

$$\begin{aligned} -(\partial_x U)p_J - D\partial_x p_J &= -(\partial_x U)p_J - D\partial_x \left[\frac{J}{D} e^{-U(x)/D} \int_x^{x_1} dy e^{U(y)/D} \right] \\ &= -(\partial_x U)p_J - J \left[-\frac{(\partial_x U)}{D} e^{-U(x)/D} \int_x^{x_1} dy e^{U(y)/D} - 1 \right] \\ &= J. \end{aligned} \quad (1.86)$$

Therefore, the inverse rate k^{-1} from Eq. (1.83) can be formally expressed as

$$k^{-1} = \frac{P_-}{J} = \frac{1}{D} \int_{-\infty}^{x_1} dx e^{-U(x)/D} \int_x^{x_1} dy e^{U(y)/D}, \quad (1.87)$$

and a partial integration yields the equivalent representation

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Assuming a sufficiently steep barrier, the integrals in Eq. (1.88) may be evaluated by adopting steepest descent approximations near the potential minimum at x_- and near the maximum at the barrier position x_b . More precisely, taking into account that $U'(x_-) = U'(x_b) = 0$, one can replace the potentials in the exponents by the harmonic approximations

$$U(x) \simeq U(x_b) - \frac{1}{2\tau_b}(x - x_b)^2,$$

$$U(y) \simeq U(x_-) + \frac{1}{2\tau_-}(y - x_-)^2,$$

where

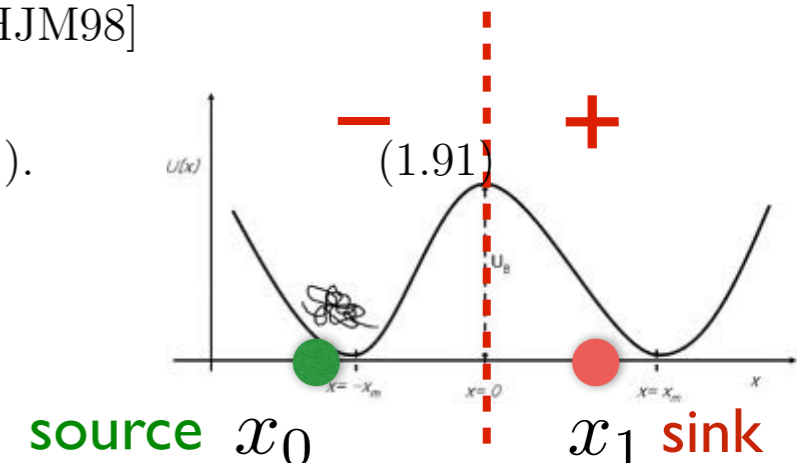
$$\tau_- = -U''(x_-) > 0, \quad \tau_b = U''(x_b) > 0 \quad (1.90)$$

carry units of time. Inserting (1.89) into (1.88) and replacing the upper integral boundaries by $+\infty$, one thus obtains the so-called Kramers rate [HTB90, GHJM98]

$$k \simeq \frac{e^{-\Delta U/D}}{2\pi\sqrt{\tau_- \tau_b}} =: k_K,$$

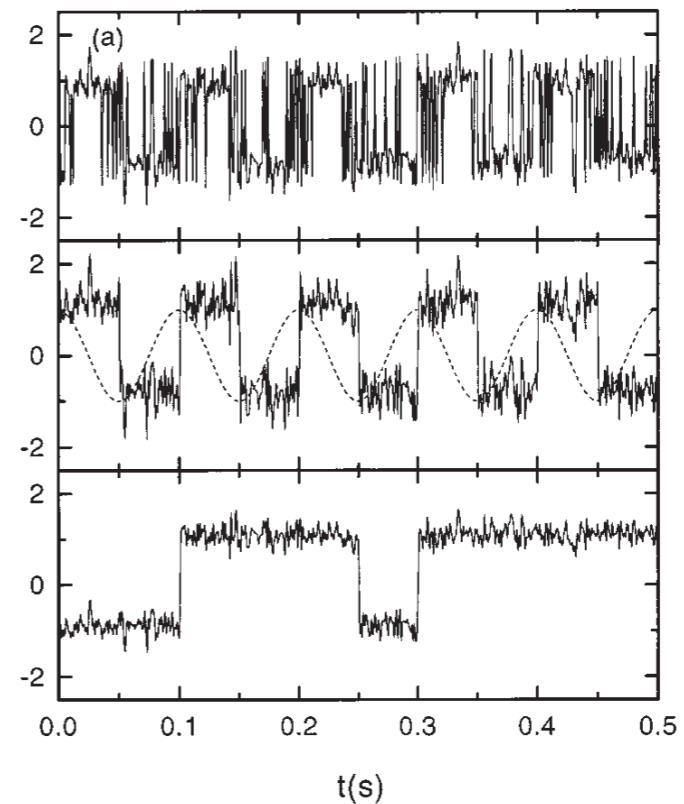
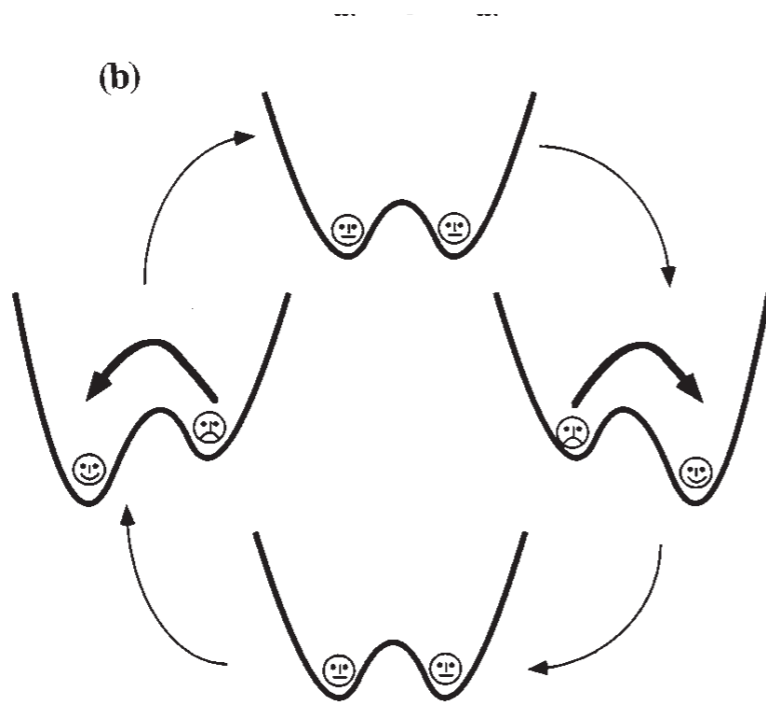
Arrhenius law

$$\Delta U = U(x_b) - U(x_-).$$



Stochastic resonance

1. a nonlinear measurement device¹⁷,
2. a periodic signal weaker than the threshold of measurement device,
3. additional input noise, uncorrelated with the signal of interest.



$$k \simeq \frac{e^{-\Delta U/D}}{2\pi\sqrt{\tau_+ \tau_b}} =: k_K \sim \Omega$$

1.5 Stochastic resonance

1.5.1 Generic model

To illustrate SR more quantitatively, consider the periodically driven SDE

$$dX(t) = -\partial_x U dt + A \cos(\Omega t) dt + \sqrt{2D} * dB(t), \quad (1.93a)$$

where A is the signal amplitude and

$$U(x) = -\frac{a}{2}x^2 + \frac{b}{4}x^4 \quad (1.93b)$$

a symmetric double-well potential with minima at $\pm x_* = \pm\sqrt{a/b}$ and barrier height $\Delta U = a^2/(4b)$. Introducing rescaled variables

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$$x' = x/x_* , \quad t' = at , \quad A' = A/(ax_*) , \quad D' = D/(ax_*^2) , \quad \Omega' = \Omega/a .$$

and dropping primes. we can rewrite (1.93a) in the dimensionless form

$$dX(t) = (x - x^3) dt + A \cos(\Omega t) dt + \sqrt{2D} * dB(t), \quad (1.93c)$$

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$$dX(t) = (x - x^3) dt + A \cos(\Omega t) dt + \sqrt{2D} * dB(t), \quad (1.93c)$$

with a rescaled barrier height $\Delta U = 1/4$. The associated FPE reads

$$\partial_t p = -\partial_x \{ [-(\partial_x U) + A \cos(\Omega t)] p - D \partial_x p \}. \quad (1.94)$$

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$$\partial_t p = -\partial_x \{ [-(\partial_x U) + A \cos(\Omega t)] p - D \partial_x p \}. \quad (1.94)$$

For our subsequent discussion, it is useful to rearrange terms on the rhs. as

$$\partial_t p = \partial_x [(\partial_x U) p + D \partial_x p] - A \cos(\Omega t) \partial_x p. \quad (1.95)$$

Perturbation theory

$$\partial_t p = \partial_x [(\partial_x U)p + D\partial_x p] - A \cos(\Omega t)\partial_x p. \quad (1.95)$$

To solve Eq. (1.95) perturbatively, we insert the series ansatz

$$p(t, x) = \sum_{n=0}^{\infty} A^n p_n(t, x), \quad (1.96)$$

which gives

$$\sum_{n=0}^{\infty} A^n \partial_t p_n = \sum_{n=0}^{\infty} \{ A^n \partial_x [(\partial_x U)p_n + D\partial_x p_n] - A^{n+1} \cos(\Omega t)\partial_x p_n \} \quad (1.97)$$

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Focussing on the linear response regime, corresponding to powers A^0 and A^1 , we find

$$\partial_t p_0 = \partial_x [(\partial_x U)p_0 + D\partial_x p_0] \quad (1.98a)$$

$$\partial_t p_1 = \partial_x [(\partial_x U)p_1 + D\partial_x p_1] - \cos(\Omega t) \partial_x p_0 \quad (1.98b)$$

Perturbation theory

$$\partial_t p = \partial_x [(\partial_x U)p + D\partial_x p] - A \cos(\Omega t) \partial_x p. \quad (1.95)$$

To solve Eq. (1.95) perturbatively, we insert the series ansatz

$$p(t, x) = \sum_{n=0}^{\infty} A^n p_n(t, x), \quad (1.96)$$

which gives

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Equation (1.98a) is just an ordinary time-independent FPE, and we know its stationary solution is just the Boltzmann distribution

$$p_0(x) = \frac{e^{-U(x)/D}}{Z_0}, \quad Z_0 = \int dx e^{-U(x)/D} \quad (1.99)$$

First-order correction

$$\partial_t p_1 = \partial_x [(\partial_x U) p_1 + D \partial_x p_1] - \cos(\Omega t) \partial_x p_0 \quad (1.98b)$$

To obtain a formal solution to Eq. (1.98b), we make use of the following ansatz

$$p_1(t, x) = e^{-U(x)/(2D)} \sum_{m=1}^{\infty} a_{1m}(t) \phi_m(x), \quad (1.100)$$

where $\phi_m(x)$ are the eigenfunctions of the unperturbed effective Hamiltonian, cf. Eq. (1.71),

$$\mathcal{H}_0 = -D \partial_x^2 + \frac{1}{4D} (\partial_x U)^2 - \frac{1}{2} \partial_x^2 U. \quad (1.101)$$

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Inserting (1.100) into Eq. (1.98b) gives

$$\sum_{m=1}^{\infty} \dot{a}_{1m} \phi_m = - \sum_{m=1}^{\infty} \lambda_m a_{1m} \phi_m - \cos(\Omega t) e^{U(x)/(2D)} \partial_x p_0. \quad (1.102)$$

First-order correction

$$\partial_t p_1 = \partial_x [(\partial_x U) p_1 + D \partial_x p_1] - \cos(\Omega t) \partial_x p_0 \quad (1.98b)$$

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Multiplying this equation by $\phi_n(x)$, and integrating from $-\infty$ to $+\infty$ while exploiting the orthonormality of the system $\{\phi_m\}$, we obtain the coupled ODEs

$$\dot{a}_{1m} = -\lambda_m a_{1m} - M_{m0} \cos(\Omega t), \quad (1.103)$$

with ‘transition matrix’ elements

$$M_{m0} = \int dx \phi_m e^{U(x)/(2D)} \partial_x p_0. \quad (1.104)$$

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The asymptotic solution of Eq. (1.103) reads

$$a_{1m}(t) = -M_{m0} \left[\frac{\Omega}{\lambda_m^2 + \Omega^2} \sin(\Omega t) + \frac{\lambda_m}{\lambda_m^2 + \Omega^2} \cos(\Omega t) \right]. \quad (1.105)$$

Note that, because $\partial_x p_0$ is an antisymmetric function, the matrix elements M_{m0} vanish¹⁸ for even values $m = 0, 2, 4, \dots$, so that only the contributions from odd values $m = 1, 3, 5 \dots$ are asymptotically relevant.

Linear response

Focussing on the leading order contribution, $m = 1$, and noting that $p_0(x) = p_0(-x)$, we can estimate the position mean value

$$\mathbb{E}[X(t)] = \int dx p(t, x) x \quad (1.106)$$

from

$$\begin{aligned} \mathbb{E}[X(t)] &\simeq A \int dx p_1(t, x) x \\ &\simeq A \int dx e^{-U(x)/(2D)} a_{11}(t) \phi_1(x) x \\ &= -AM_{10} \left[\frac{\Omega}{\lambda_1^2 + \Omega^2} \sin(\Omega t) + \frac{\lambda_1}{\lambda_1^2 + \Omega^2} \cos(\Omega t) \right] \int dx e^{-U(x)/(2D)} \phi_1(x) x \end{aligned}$$

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Using $\lambda_1 = 2k_K$, where k_K is the Kramers rate from Eq. (1.91), we can rewrite this more compactly as

$$\mathbb{E}[X(t)] = \bar{X} \cos(\Omega t - \bar{\varphi}) \quad (1.107a)$$

with phase shift

$$\bar{\varphi} = \arctan\left(\frac{\Omega}{2k_K}\right) \quad (1.107b)$$

and amplitude

$$\bar{X} = -A \frac{M_{10}}{(4k_K^2 + \Omega^2)^{1/2}} \int dx e^{-U(x)/(2D)} \phi_1(x) x. \quad (1.107c)$$

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The amplitude \bar{X} depends on the noise strength D through k_K , through the integral factor and also through the matrix element

$$M_{10} = \int dx \phi_1 e^{U(x)/(2D)} \partial_x p_0. \quad (1.108)$$

To compute \bar{X} , one first needs to determine the eigenfunction ϕ_1 of \mathcal{H}_0 as defined in Eq. (1.101). For the quartic double-well potential (1.93b), this cannot be done analytically but there exist standard techniques (e.g., Ritz method) for approximating ϕ_1 by functions that are orthogonal to $\phi_0 = \sqrt{p_0/Z_0}$. Depending on the method employed, analytical

Linear response

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$$\bar{X} \simeq \frac{Aa}{Db} \left(\frac{4k_{\text{K}}^2}{4k_{\text{K}}^2 + \Omega^2} \right)^{1/2}, \quad (1.109)$$

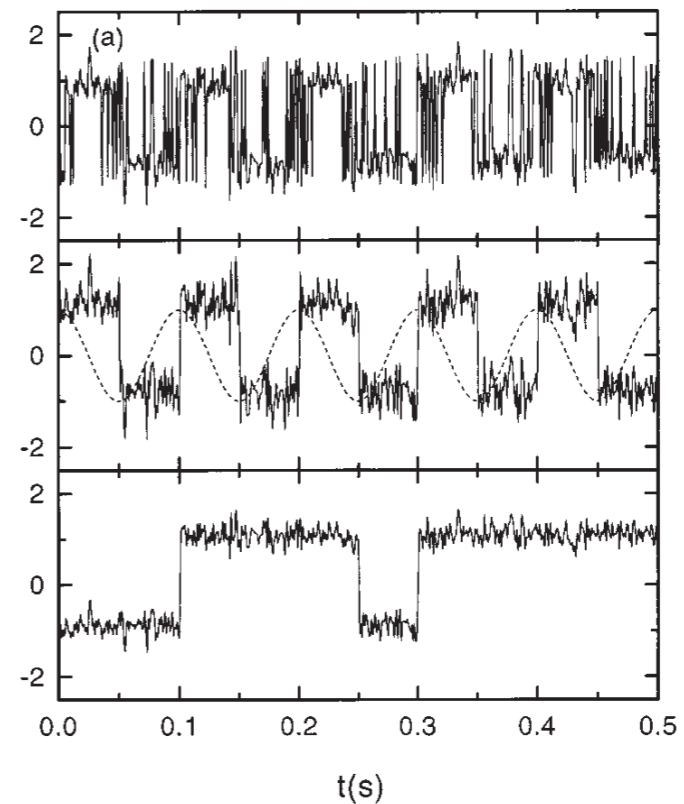
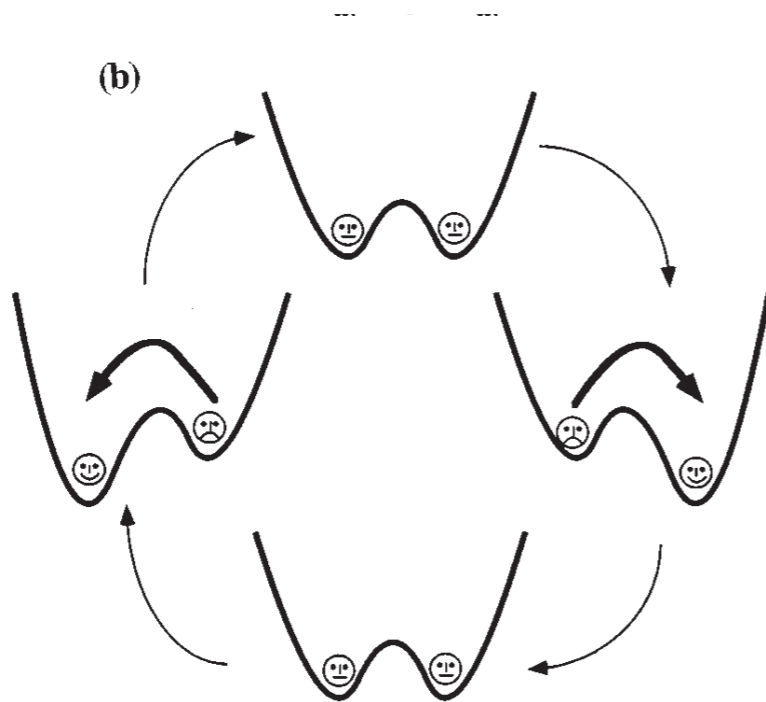
which exhibits a maximum for a critical value D_* determined by

$$4k_{\text{K}}^2 = \Omega^2 \left(\frac{\Delta U}{D_*} - 1 \right). \quad (1.110)$$

That is, the value D_* corresponds to the optimal noise strength, for which the mean value $\mathbb{E}[X(t)]$ shows maximal response to the underlying periodic signal – hence the name ‘stochastic resonance’ (SR).

Stochastic resonance

1. a nonlinear measurement device¹⁷,
2. a periodic signal weaker than the threshold of measurement device,
3. additional input noise, uncorrelated with the signal of interest.



$$k \simeq \frac{e^{-\Delta U/D}}{2\pi\sqrt{\tau_+ \tau_b}} =: k_K \sim \Omega$$

1.5.2 Master equation approach

Similar to the case of the escape problem, one can obtain an alternative description of SR by projecting the full FPE dynamics onto a simpler set of master equations for the probabilities $P_{\pm}(t)$ of the coarse-grained particle-states ‘left well’ ($-$) and ‘right well’ ($+$), as defined by Eq. (1.76). This approach leads to the following two-state master equations with time-dependent rates

$$\dot{P}_-(t) = -k_+(t) P_- + k_-(t) P_+, \quad (1.111a)$$

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The general solution of this pair of ODEs is given by [GHJM98]

$$P_{\pm}(t) = g(t) \left[P_{\pm}(t_0) + \int_{t_0}^t ds \frac{k_{\pm}(s)}{g(s)} \right] \quad (1.112a)$$

where

$$g(t) = \exp \left\{ - \int_{t_0}^t ds [k_+(s) + k_-(s)] \right\}. \quad (1.112b)$$

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To discuss SR within this framework, it is plausible to postulate time-dependent Arrhenius-type rates,

$$k_{\pm}(t) = k_K \exp \left[\pm \frac{Ax_*}{D} \cos(\Omega t) \right]. \quad (1.113)$$

Considering the asymptotic limit $t_0 \rightarrow -\infty$, one can Taylor-expand the rates for $Ax_* \ll D$ to obtain

$$k_{\pm}(t) = k_{\text{K}} \left[1 \pm \frac{Ax_*}{D} \cos(\Omega t) + \left(\frac{Ax_*}{D} \right)^2 \cos^2(\Omega t) \pm \dots \right]$$

These approximations are valid for slow driving (adiabatic regime), and they allow us to compute expectation values to leading order in Ax_*/D . To first order, one then finds for the conditional probability

$$\begin{aligned} P_+(t|x_0, t_0) &= 1 - P_-(t|x_0, t_0) \\ &= \frac{1}{2} \left\{ e^{-2k_{\text{K}}(t-t_0)} [2\delta_{x_0, x_*} - 1 - \kappa(t_0)] + 1 + \kappa(t) \right\} \end{aligned} \quad (1.114a)$$

where

$$\kappa(t) = \frac{Ax_*}{D} \cos(\Omega t - \bar{\varphi}) \left(\frac{4k_{\text{K}}^2}{4k_{\text{K}}^2 + \Omega^2} \right)^{1/2}, \quad \bar{\varphi} = \arctan\left(\frac{2\Omega}{k_{\text{K}}}\right). \quad (1.114b)$$

Note that the conditional probability $P_+(t|x_0, t_0)$ satisfies the initial condition

$$P_+(t_0|x_0, t_0) = \delta_{x_0, x_*} = \begin{cases} 1, & x_0 = x_* \\ 0, & \text{otherwise} \end{cases}, \quad (1.115)$$

where $x_* = x_{\pm}$ depending on whether the particle starts in the left or right well. Furthermore, one then finds for the mean position the asymptotic linear response result [GHJM98]

$$\mathbb{E}[X(t)] = \bar{X} \cos(\Omega t - \bar{\varphi}) \quad (1.116a)$$

where

$$\bar{X} = \frac{Ax_*^2}{D} \left(\frac{4k_{\text{K}}^2}{4k_{\text{K}}^2 + \Omega^2} \right)^{1/2}, \quad \bar{\varphi} = \arctan\left(\frac{\Omega}{2k_{\text{K}}}\right). \quad (1.116b)$$

Note that Eqs. (1.116) are consistent with our earlier result (1.107).