Chapter 7
Control and Energetics

For a system external agents act as a main source of free energy, on one hand, and also as agents that control the processes, on the other hand. For example, when one drives a car, the car (system) needs two kinds of external agents; fuels (oil and oxygen) and a driver. From the viewpoint of energetics, the work for controlling the processes of a macroscopic system is usually negligible as compared with the main work, such as the combustion of fuel to keep a car going. It is, therefore, reasonable that standard textbooks of thermodynamics describe the Carnot heat engine without mentioning the work of attaching or detaching the engine with the heat baths.

In fluctuating mesoscopic systems, however, the situation is different. The work to control a fluctuating system can be an important part of the total work exchanged between the system and its external agents. Ignorance of this type of work would easily lead to paradoxes. If one were to invent a perpetual machine, and if one would check the consistency of this machine with the second law of thermodynamics, it would be better to make a mesoscopic model, because the energetics of control appears naturally in the mesoscopic description.

There have been many studies on the work related to control:

- *Paradox of Maxwell's demon [1]:* the "demon" which makes use of thermal fluctuations to realize a perpetual machine of the second kind (see Sect. 4.2.1.2).
- *Thermodynamics of computation [2, 3]:* theories revealing the minimal irreversible work to operate a binary digit memory (Sect. 7.1.2 below).
- *Feynman ratchet and pawl [4]:* a model of autonomous heat engine (see Sect. 1.3.4.2).
- *Motor proteins [5]:* autonomous chemical engines of molecular scale, such as linear or rotatory molecular motors or ion pumps. (See Chap. 8).
- *Signal transducing proteins [6]:* G-proteins, etc., which share a universal molecular architecture with the motor proteins [7].

One of the main questions about the energetics of control is "Can any type of operations to a system be done quasistatically?" (Sect. 7.1), because we know that quasistatic work is recoverable. Among the processes of control, there are certain important cases where the process can never be done quasistatically *by construction*. We will call such processes *essentially nonquasistatic processes*. There are two

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distinct mechanisms that disable a quasistatic process, and these two mechanisms come into play often together:

(Case 1) *The operation of external system imposes the crossover of timescales between the system's relaxation time and the time taken for the operation* (Sect. 7.1.1). Irreversible work directly associated with such operations can, however, be reduced as small as we want.

(Case 2) *A system loses the information about its past history when a system becomes equilibrated with a new environment* (Sect. 7.1.3). This type of nonquasistatic process costs certain irreversible work irrespective of the time of operation. Or, at least up to now we do not know how to reduce the irreversible work.

In 1960s Landauer [2], Bennett [3], and others have elucidated the minimal irreversible work required for a cycle of operations on a single-bit memory. While the operation of a single-bit memory includes essentially nonquasistatic processes of (Case 1), this minimal irreducible work and the above mentioned reducible irreversible work should be distinguished (Sect. 7.1.2).

The control of free-energy transducers will be discussed separately in Chap. 8.

Another important question of control concerns detection under fluctuations (Sect. 7.2). How can a mesoscopic system detect external signal particles with maximum certainty and minimum cost? While a "gate" correlates actively the objects of control with the subject system, the "sensor" or detector correlates passively the system with its surroundings. The two principles for avoiding the thermal noises from the detection use, respectively, (i) the steric repulsion or (ii) the compensation of interaction energies.

7.1 Limitations of Quasistatic Operations

*7.1.1 * Essentially Nonquasistatic Process is Generally Caused by Crossover of Timescales τ_{op} and τ_{sys}*

7.1.1.1 Two Timescales, τ_{op} and τ_{sys}

We will use the term *operations* to mean generically control and observation. The timescale of operations has an upper limit, as well as a lower limit (i.e., the time resolution). The upper limit is often the maximal time of tolerance, or the timescales beyond which the constituting elements of the system become unstable (see Sects. 1.3.3.1 and 3.1.1). We denote by τ_{op} this upper limit timescale.[1] The effect of operation on a system depends on the relaxation time of the system. We

[1] The "op" is for operation.

denote by τ_{sys} this time. The ratio between these two timescales is sometimes called the Deborah number, $De \equiv \tau_{\mathrm{sys}}/\tau_{\mathrm{op}}$.

7.1.1.2 Crossover of Timescales

The crossover of timescales is the phenomenon that the relative magnitudes of τ_{sys} and τ_{op} change between $\tau_{\mathrm{sys}} \gg \tau_{\mathrm{op}}$ and $\tau_{\mathrm{sys}} \ll \tau_{\mathrm{op}}$ (see Fig. 7.1) during an operation. More precisely,

(i) The relaxation time of the system, $\tau_{\mathrm{sys}}(a)$, depends on the system parameter, a.
(ii) During a characteristic time of operation, τ_{op}, an external system changes the value of a.
(iii) The change in a is such that the relaxation time $\tau_{\mathrm{sys}}(a)$ changes from the full relaxation regime, $\tau_{\mathrm{sys}}(a) \ll \tau_{\mathrm{op}}$, to the regime of "freezing", $\tau_{\mathrm{sys}}(a) \gg \tau_{\mathrm{op}}$, or the inverse. (Fig. 7.1 *right*)

This operation is, by definition, nonquasistatic. Especially, if $\tau_{\mathrm{sys}}(a_{\mathrm{f}}) = \infty$ at the end of the operation (Fig. 7.1 *left*), whatever large τ_{op} cannot satisfy the quasistatic condition $\tau_{\mathrm{sys}}(a) \ll \tau_{\mathrm{op}}$ throughout the operation.

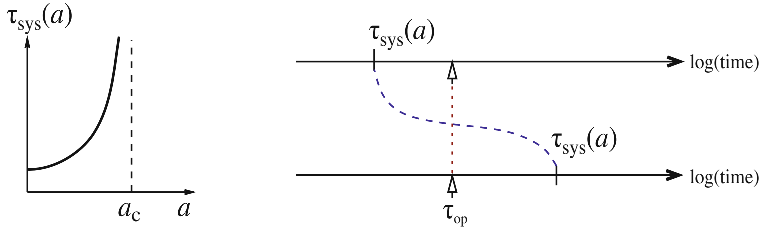

Fig. 7.1 (*Left*) $\tau_{\mathrm{sys}}(a)$ vs. a. The figure shows the case where $\tau_{\mathrm{sys}}(a)$ diverges for $a \uparrow a_c$. (*Right*) Change of $\tau_{\mathrm{sys}}(a)$ across the operation time τ_{op} through the change of parameter a. The time axes should be regarded as logarithmic scale

7.1.1.3 Barrier Height and Relaxation Time

Let us look at a simple example of the crossover of timescales. The system is a single Brownian particle in the force potential $U(x,a)$ (see Fig. 7.2) and confined in a finite zone Ω_{tot} with $-L/2 \le x \le L/2$. Inside Ω_{tot} the potential energy $U(x,a)$ depends on the parameter a only in a small zone Ω of the width $|\Omega| = \delta(< L)$. Outside this zone, we assume that $U(x,a)$ =const. for any value of a. For simplicity we assume the symmetry, $U(-x,a) = U(x,a)$, with the maximum being located at $x = 0$.

The Brownian particle obeys the Langevin equation,

$$0 = -\frac{\partial U(x,a)}{\partial x} - \gamma \frac{dx}{dt} + \xi(t) \qquad (x \in \Omega_{\mathrm{tot}}). \tag{7.1}$$

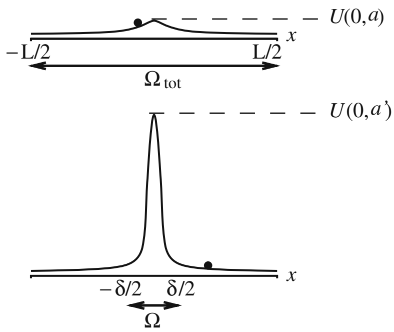

Fig. 7.2 A Brownian particle (*thick black dot*) in a zone $\Omega_{\rm tot} \equiv \{x| - L/2 \le x \le L/2\}$ along the x-axis. The curves show the profiles of the potential energy $U(x,a)$ with $a_{\rm i} \le a < a^*$ (*top*) and $U(x,a')$ with $a^* < a' \le a_{\rm f}$ (*bottom*) vs. x. The maximum value of the potential is $U(0,a) \sim k_{\rm B}T$ and $U(0,a') \gg k_{\rm B}T$, respectively. The profile of the potential $U(x,a)$ changes only in the zone, $\Omega \equiv \{x| - \delta/2 \le x \le \delta/2\}$

If the height of the potential barrier, $U(0,a)$, is small, i.e., $U(0,a)/k_{\rm B}T \sim 1$, the time $\tau_{\rm sys}$ is approximately the diffusion time, $\tau_0 \equiv L^2/(2D)$ $(D = k_{\rm B}T/\gamma)$, for a Brownian particle to visit almost entire zone $\Omega_{\rm tot}$. By contrast, if $U(0,a)/k_{\rm B}T \gg 1$ the relaxation time of the system, $\tau_{\rm sys}(a)$, is essentially the inverse rate of thermally activated transition across the potential barrier. According to (3.40) the rate is roughly given by

$$\frac{1}{\tau_{\rm sys}(a)} \equiv \frac{1}{\tau_0} e^{-\frac{U(0,a)}{k_{\rm B}T}}, \tag{7.2}$$

where we have ignored the corrections in the prefactor due, for example, to the details of the potential profile.

Now suppose that $U(0,a_{\rm i}) \sim k_{\rm B}T$ for the initial value $a_{\rm i}$ and $U(0,a_{\rm f}) \gg k_{\rm B}T$ for the final value $a_{\rm f}$. Then $\tau_{\rm sys}(a)$ increases from $\tau_{\rm sys}(a_{\rm i})/\tau_0 \sim 1$ to $\tau_{\rm sys}(a_{\rm f})/\tau_0 \gg 1$ during the operation time $\tau_{\rm op}$. For example, if $\tau_0 = 10^{-9}$s and $\tau_{\rm op} = 1$ h, the crossover point $\tau_{\rm sys}(a) \sim \tau_{\rm op}$ is attained for $U(0,a) \sim 30k_{\rm B}T$. In the regime of $\tau_{\rm sys}(a) \gg \tau_{\rm op}$ the particle is practically localized within either side of the potential barrier. Through the crossover of the timescales, the accessible phase space of the system shrinks almost discontinuously. Moreover, we cannot precisely predict which subspace the particle will be confined to. The probabilities that the particle is confined to the left $(x < 0)$ and that to the right $(x > 0)$ of the barrier are 1/2:1/2.

7.1.1.4 Work to Raise the Potential Barrier

Essentially nonquasistatic process does not necessarily imply a large irreversible work. We will show that the *irreversible* part of the work associated with raising the potential barrier of Fig. 7.2 can be made very small if we carefully choose a protocol of raising the potential barrier.[2] We will denote by a^* ($a_\mathrm{i} < a^* < a_\mathrm{f}$) the value of the parameter a at the crossover of timescales, i.e., $\tau_\mathrm{sys}(a^*) \simeq \tau_\mathrm{op}$.[3] For $a_\mathrm{i} \le a(t) < a^*$ the almost quasistatic operation is realizable while for $a^* < a(t) \le a_\mathrm{f}$ it is impossible in any case because $\tau_\mathrm{sys}(a(t)) \gg \tau_\mathrm{op}$.

The optimal strategy to minimize the irreversible work is that we spend most of the operation time in raising the potential barrier up to $U(0, a^*)$ so that the associated work is almost recoverable when the barrier will be lowered. During this stage, the probability density $\mathcal{P}(x,t)$ for the particle position x is close to the canonical distribution over the entire zone Ω_tot, $\mathcal{P}^\mathrm{eq}(x,a;T) = e^{[F(a,T)-U(x,a)]/k_\mathrm{B}T}$, where $e^{-F(a,T)/k_\mathrm{B}T} \equiv \int_{\Omega_\mathrm{tot}} e^{-U(x,a)/k_\mathrm{B}T}dx$. The associated (almost quasistatic) work $W_{[a_\mathrm{i},a^*]}$ is (see (4.6))

$$W_{[a_\mathrm{i},a_*]} \simeq F(a^*,T) - F(a_\mathrm{i},T). \tag{7.3}$$

The error in (7.3), i.e., the irreversible work associated with this slow process, is approximately proportional to the inverse of the time spent, i.e., $\sim \tau_\mathrm{op}{}^{-1}$, as discussed in Sect. 5.3.1.

After this almost quasistatic work, we will raise the barrier height from $U(0, a^*)$ to $U(0, a_\mathrm{f})$ in a short time. The average work $\langle W\rangle_{[a^*,a_\mathrm{f}]}$ associated with this step during $a^* < a(t) \le a_\mathrm{f}$ is estimated to be

$$\frac{\langle W\rangle_{[a^*,a_\mathrm{f}]}}{k_\mathrm{B}T} \le \frac{(\mathrm{const.})\delta}{L} e^{-U(0,a^*)/k_\mathrm{B}T}\,\frac{U(x,a_\mathrm{f}) - U(x,a^*)}{k_\mathrm{B}T}, \tag{7.4}$$

Leaving the derivation to Appendix A.7.1, the result (7.4) can be qualitatively explained: Since the height of the potential barrier $U(0, a^*)$ is already very large with respect to $k_\mathrm{B}T$, the particle almost surely escapes from the region Ω where the barrier is rising. Therefore, in most cases virtually no work is needed to raise the barrier. However, in rare cases, with the probability of $\sim (\delta/L)\, e^{-U(0,a^*)/k_\mathrm{B}T}$, a particle happens to remain within the zone Ω and is "lifted up." The last process costs the work of the order of $U(0, a_\mathrm{f}) - U(0, a^*)$. Therefore, we have (7.4). The last work is not recoverable because in the reverse operation from a_f to a^*, the probability to find the particle within Ω at $a = a_\mathrm{f}$ is extremely less than $\mathcal{P}^\mathrm{eq}(x, a^*; T)$.

Equation (7.4) tells that $\langle W\rangle_{[a^*,a_\mathrm{f}]}/k_\mathrm{B}T$ can be made very small due to the exponential factor, $e^{-U(0,a^*)/k_\mathrm{B}T}$. If we take $\tau_0 = 10^{-13}$ s and $U(0, a_\mathrm{f})/k_\mathrm{B}T \simeq 10^3$, then $\tau_\mathrm{op} = 1$ ms is sufficient to satisfy $\langle W\rangle_{[a^*,a_\mathrm{f}]}/k_\mathrm{B}T < 10^{-7}$. That is, we need the *irreversible* work of less than 10^{-5}% of $k_\mathrm{B}T$ and the time of 1 ms to establish the barrier which a particle will not pass before $\tau_0 e^{U(0,a^*)/k_\mathrm{B}T} > 10^{400}$ days. Moreover,

[2] We discuss here about the irreversible work being *directly* related to a single action of raising the barrier: This work should be distinguished from the irreversible work associated with the cyclic operation to erase a single-bit memory. See Sect. 7.1.2.

[3] Practically, it is better to include a "safety factor" to define $\tau_\mathrm{sys}(a^*)/\tau_\mathrm{op} \simeq 10 - 10^2$ rather than $\tau_\mathrm{sys}(a^*)/\tau_\mathrm{op} \simeq 1$. We, however, ignore this point for the simplicity of the argument.

this $10^{-7}k_BT$ of work is not typical work: for the most realizations, W is practically 0 ($\ll 10^{-7}$), while for one realization out of $e^{10^3} \sim 10^{430}$ the work is $W \sim 10^3 k_BT$.

The access of particles to an open system from particle environments (reservoirs) can be controlled by the gates which consist of variable potential barriers between the system and the reservoirs.[4] The crossover of timescales of the type (1), therefore, occurs inevitably whenever the open system is attached or detached with particle environments.

7.1.1.5 Attachment/Detachment with a Thermal Environment

Attaching or detaching a (closed) system with a thermal environment also causes the crossover of timescales. When a system is in contact with a thermal environment of temperature T, the system's energy undergoes temporal fluctuations. From the viewpoint of energetics, the relaxation time of a system, $\tau_{\rm sys}$, is the time over which the temporal history of the system's energy approaches the canonical distribution. If the system is completely detached from its thermal environment, the system's energy becomes fixed. The relaxation time, $\tau_{\rm sys}$, is then infinite. Therefore, the operation of detaching a system from its thermal environment inevitably causes crossover of timescales.

Can we calculate the work associated with attachment/detachment with a thermal environment? In the Langevin equation (7.1) only the parameter γ characterizes the interaction between the system and its thermal environment.[5] One might regard γ as an externally controlled parameter. But the framework of stochastic energetics has excluded the control of the interface between a system and thermal environments (Sect. 4.1.1.1). A way to go around this constraint is schematically shown in Fig 7.3. We will call this device the "clutch mechanism." We introduce an auxiliary degree of freedom, say y, which always stays in contact with a thermal environment, and whose fluctuating motion is described by a Langevin equation. The variable of the main system, say x, does not interact any more with thermal environments, but it interacts with this auxiliary degree of freedom, y, through an interaction potential energy, say $\phi(x, y, \chi)$, where χ is the control parameter of operation.[6] One may interpret that the auxiliary variable y stands for those fluctuation modes of the thermal environment which is coupled to the system variable x.[7] The system of Langevin equations is

$$\frac{dx}{dt} = \frac{p}{m}, \qquad \frac{dp}{dt} = -\frac{\partial U(x,a)}{\partial x} - \frac{\partial \phi(x,y,\chi)}{\partial x}, \tag{7.5}$$

[4] Sect. 7.2.2 below.

[5] Remember that the random force $\xi(t)$ is also characterized by $\gamma k_B T$.

[6] We reserve a for the control parameter of the main system.

[7] See the discussion at the end of Sect. 6.3.2.

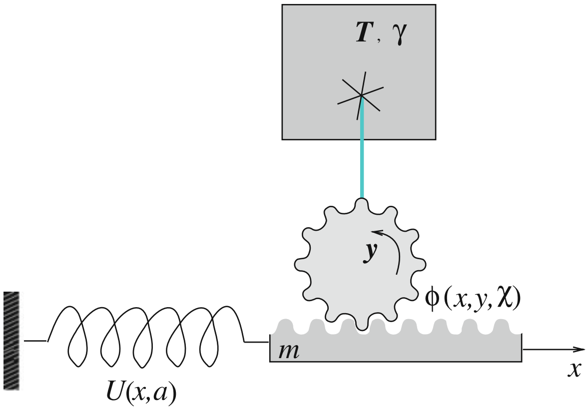

Fig. 7.3 A clutch mechanism to attach/detach a system with a thermal environment using an auxiliary variable y and an interaction potential $\phi(x, y, \chi)$

$$0 = -\gamma \frac{dy}{dt} + \xi(t) - \frac{\partial \phi(x, y, \chi)}{\partial y}. \tag{7.6}$$

In (7.6) and in Fig 7.3 we assumed that y is a rotational degree of freedom (i.e., angle) so that its Brownian motion is confined within a periodic domain of period 2π. We assume $\phi(x, y, \chi)$ such that (see Fig 7.4) for $\chi = 0$ there is no energetic coupling between x and y, i.e., $\phi(x, y, 0) = 0$, and for $\chi = 1$ the variation of y is highly correlated with that of x. For $0 < \chi < 1$, change of $\phi(x, y, \chi)$ is supposed to be monotonous with χ.

When the parameter χ is decreased down to the decoupling limit $\chi = 0$, the crossover of timescales is unavoidable with whatever large τ_{op}.[8] We will use the clutch mechanism to model the Carnot heat engine (Sect. 8.1.1) and the total work to operate χ parameters will be calculated in Sect. 8.1.1.2.

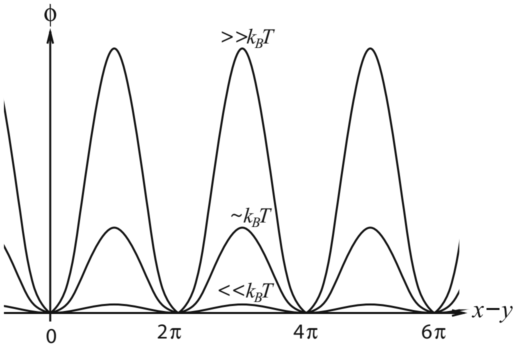

Fig. 7.4 Potential function used for the clutch mechanism, $\phi(x, y, \chi)$ vs. $x - y$, is shown for $\chi \simeq 0$ (*bottom curve*), $0 < \chi < 1$ (*middle curve*), and $\chi = 1$ (*top curve*)

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[8] There is a secondary crossover of timescales in the opposite limit, $\chi \to 1$ if $\phi(x, y, 1) \gg k_{\mathrm{B}}T$. For high barriers, the slippage between the variations of x and y is blocked.

7.1.1.6 Remarks

Generality of the Crossover of Timescales and Spatial Scales

Figure 7.2 represents a naïve oversimplified picture of the glass transition, where lowering temperature or changing other fields splits the equilibrium states into more than one (meta) stable states.

The crossover of timescales has long been known in quantum chemistry. The Born–Oppenheimer approximation assumes that the electrons' state follows quickly enough the movement of atoms or ions [8]. But when the two atoms are gradually separated, the rate of the electronic transition between the atoms becomes smaller and smaller with the increase of the interatomic distance. Therefore, the timescale of the electronic transition diverges during this process. Eventually the Born–Oppenheimer approximation becomes invalid.

The crossover of spatial scales has been studied in quantum mechanics. The Wentzel–Kramers–Brillouin (WKB) approximation [9] assumes that the de Broglie wavelength of the particle, $2\pi/k$, is much shorter than the length scale over which this wavelength varies. The de Broglie wavelength depends on the total energy E and the potential energy $U(x)$ through $\hbar k = \sqrt{2m(E - U(x))}$, where $\hbar$ is the Planck constant/2π and m is the mass of the particle. The *turning point* x^* is defined by $E = U(x^*)$. At this point the de Broglie wavelength diverges. The WKB approximation becomes, therefore, inevitably invalid as x approaches the turning point.

Auto-Adjusting Timescales

In the above examples the timescales are controlled by external operations. When the system's relaxation time $\tau_{\rm sys}$ depends on the system's state, $\tau_{\rm sys}$ can be adjusted by itself in the vicinity of the timescale of operation $\tau_{\rm op}$. A very simple model of aging and plastic flow show that $\tau_{\rm sys}$ approaches to $\tau_{\rm op}$ from below and from above, respectively. The models are described in Appendix A.7.2.

Consequences of the Discontinuous Change of Accessible Phase Space

As shown in Sect. 7.1.1.4, the irreversible work related to the crossover of timescales can be made small by suitably choosing the protocol of operation. Then what is the major outcome of this type of essentially nonquasistatic process?

The answer concerns the change of accessible phase spaces for the system. The final state of the system is confined to a subset of phase space which has been entirely available before. The reduction of accessible phase space contains the memory of either the external operation or the fluctuations in the environment when the crossover of the timescale took place. This memory can have an influence on the subsequent response of the system. In the following Sect. 7.1.2 we describe the irreversible work to operate a single-bit memory as a typical example.

7.1.2 Minimal Cost of the Operation of Single-Bit Memory is Related to the Second Law

Operation of a single-*bit* (binary digit) memory uses the crossover of timescales. The objects of the present section are:

I. To give a physical expression of the memory: A bit memory is a physical state of the system. This information can be changed as a physical process, either through the operations by the external system or through the fluctuations due to the interaction with the environment.
II. To relate the irreversible loss of information with the irreversible work: For a bit memory, the cyclic operation of *overwriting* is a basic physical process. Its energetics is described.
III. To describe "to know" in physics' language (Sect. 7.1.2.3): The process of copying the information is analyzed, including its minimal cost.

The basis of this subject was founded by Landauer [2] and Bennett [3] (see a survey [1]). They have shown that the work of overwriting a memory is no less than the work which "Maxwell's demon" can extract. Therefore, no perpetual machine of the second kind can be constructed on the basis of memory operations. Stochastic energetics provides an explicit formulation of the minimal irreversible work along a single realization of memory operation.

7.1.2.1 A Model of Bit Memory Operations

A single-bit memory is realized by a state point ("particle"), x, within a double-well potential, $U(x, a, b)$. See Fig. 7.5.

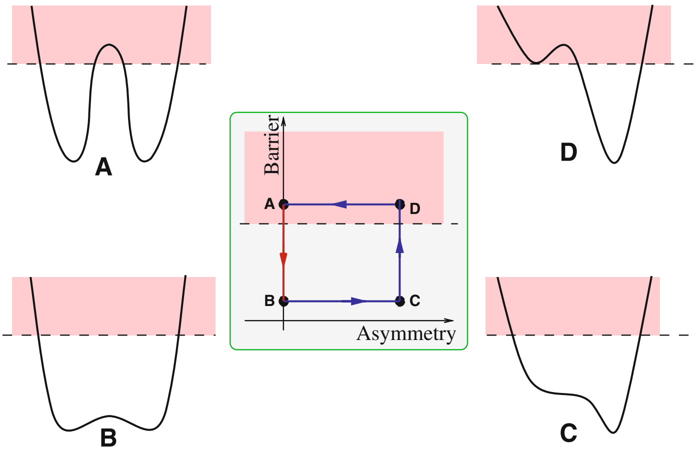

Fig. 7.5 A cycle of operation of overwriting, which consists of the erasure, $\mathcal{E}$: A $\to$ B, and the subsequent writing, $\mathcal{W}$: B $\to$ C $\to$ D $\to$ A

The particle is in contact with a thermal environment at temperature T. Neglecting the inertia effect, x obeys the following Langevin equation:

$$\gamma \frac{dx}{dt} = -\frac{\partial U(x, a, b)}{\partial x} + \xi(t), \tag{7.7}$$

where γ is the friction coefficient, $\xi(t)$ is the white Gaussian process of zero mean with $\langle \xi(t)\xi(t')\rangle = 2\gamma k_{\mathrm{B}} T \delta(t - t')$. The operation requires two parameters, a and b [2]. The parameter a controls the <u>a</u>symmetry of the potential to bias the memory to take a desired state, while the parameter b controls the <u>b</u>arrier height of the potential. $U(x, a, b) = -ax + b(x^2 - 1)^2$ is an example.

We split the x-axis into the left half $\Omega_0 = (-\infty, 0)$ and the right half $\Omega_1 = (0, \infty)$. Then the states $\sigma = 0$ [$\sigma = 1$] of the memory are assigned to $x \in \Omega_0$ [$x \in \Omega_1$], respectively.

By the dashed horizontal line and the shaded zone in Fig. 7.5 A–D, we denote the zone of (free) energy which the particle practically never attains within τ_{op} if it starts from the minimum of the potential. For example, in Fig 7.5A, the particle remains within one of the valleys, that is, the state of the memory σ is stable. Likewise, in Fig 7.5D the memory is in $\sigma = 1$ state. By contrast, in Fig 7.5B, C, the system's relaxation time τ_{sys} is less than τ_{op}. The memory σ can flip between 0 and 1.

The counterclockwise cycle in Fig. 7.5, A→B→C→D→A, is the operation of overwriting. This operation is decomposed into the process of erasing memory, $\mathcal{E}$, and the process of writing memory, $\mathcal{W}$:

$$\begin{aligned} \text{Erasing, } \mathcal{E}: &\quad \mathrm{A} \to \mathrm{B}, \\ \text{Writing, } \mathcal{W}: &\quad \mathrm{B} \to \mathrm{C} \to \mathrm{D} \to \mathrm{A}. \end{aligned} \tag{7.8}$$

Suppose that the system has retained a memory state, σ, in A. Through the process $\mathcal{E}$, this memory is lost. Then by the process $\mathcal{W}$, the memory is forcedly reset to the state $\sigma = 1$. In order to reset to the state $\sigma = 0$, the profiles of C and D should be replaced by their mirror images C* and D*, respectively.

The Timescales and Branching of Protocol

In Fig. 7.5 the operations A $\leftrightarrow$ B and A $\leftrightarrow$ D are the essentially nonquasistatic processes, as discussed in Sects. 7.1.1.2. Through these transitions, the accessible phase space for $x(t)$ changes discontinuously.

To look at the timescales more systematically, let us introduce two relaxation times: $\tau_{\mathrm{sys}}^{(0\to 1)}$ associated with the transition of σ from 0 to 1, and $\tau_{\mathrm{sys}}^{(1\to 0)}$ from 1 to 0. Therefore, four situations are possible with respect to the timescales:

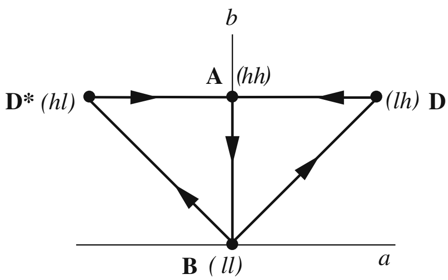

Fig. 7.6 The cycles of overwriting process viewed from the timescales. See the text

$$
\begin{aligned}
(hh)&: \tau_{\rm sys}^{(0\to 1)}/\tau_{\rm op} \gg 1 \quad \text{and} \quad \tau_{\rm sys}^{(1\to 0)}/\tau_{\rm op} \gg 1\\
(h\ell)&: \tau_{\rm sys}^{(0\to 1)}/\tau_{\rm op} \gg 1 \quad \text{and} \quad \tau_{\rm sys}^{(1\to 0)}/\tau_{\rm op} \ll 1\\
(\ell h)&: \tau_{\rm sys}^{(0\to 1)}/\tau_{\rm op} \ll 1 \quad \text{and} \quad \tau_{\rm sys}^{(1\to 0)}/\tau_{\rm op} \gg 1\\
(\ell\ell)&: \tau_{\rm sys}^{(0\to 1)}/\tau_{\rm op} \ll 1 \quad \text{and} \quad \tau_{\rm sys}^{(1\to 0)}/\tau_{\rm op} \ll 1. \qquad (7.9)
\end{aligned}
$$

Now the two control parameters (a, b) are essentially reflected in $\ln[\tau_{\rm sys}^{(0\to 1)}/\tau_{\rm sys}^{(1\to 0)}]$ and $\ln[\tau_{\rm sys}^{(0\to 1)}\tau_{\rm sys}^{(1\to 0)}/\tau_{\rm op}^2]$, respectively. Therefore, the operations of overwriting and the timescales can be related as shown in Fig. 7.6. In this schema, the important part of the cycle is the vertical process, A→B. While the external system does the same operation along $a = 0$ line, the memory state at A depends on the previous operation, either from D or from D*. Therefore, it is often said that this erasure process $\mathcal{E}$ is the origin of irreversibility.

7.1.2.2 Energetics of the Writing and Erasure of a Bit Memory

Hereafter we consider only slow operations to change a and b.[9] Then we ignore the irreversible work of almost quasistatic process. Also, we ignore the irreversible work directly associated to the essentially nonquasistatic operations based on the argument in Sect. 7.1.1.4.

Irreversibility of the Operation of Overwriting

If we do the erasing process $\mathcal{E}$ and immediately retrace it, i.e., A→B→A, there is practically no irreversible work. The same is true if we do the writing process $\mathcal{W}$ and immediately retrace it, i.e., B→C→D→A→D→C→B, because the state is definitely $\sigma = 1$ at the turning stage A. Furthermore, if we do the sequential processes, $\mathcal{E} \to \mathcal{W}$, and immediately retrace them in the reverse order, i.e., A→B→C→D→A→D→C→B→A, there is no irreversible work. One might then expect that any process along this circle is reversible. In fact it is not the case. For example, along the path B→C→D→A→B→A→D →C→B, the external

[9] cf. Sect. 5.3.1.

system loses control of the state σ after the process, A$\to$B, as discussed in the above. If upon the operation of B$\to$A the memory comes back to $\sigma = 0$, then the subsequent operations, A$\to$D$\to$C$\to$B, will cost a work much more than $k_{\mathrm{B}}T$. This is an example of the consequence of the discontinuous change of accessible phase space (Sect. 7.1.1.6).

Furthermore, we will see below that the total work for the overwriting, A$\to$B$\to$C$\to$D$\to$A, is nonzero, bounded below by $k_{\mathrm{B}}T \ln 2$ per cycle.

Estimation of the Work of Writing: $\mathcal{W}$

The operation B$\to$C$\to$D can be done quasistatically. Also the operation D$\to$A costs no work since, after the process B$\to$C$\to$D, the state is surely $\sigma = 1$. In the last process, D$\to$A, the potential energy $U(x, a, b)$ can, therefore, be replaced by an effective potential $U^{\mathrm{eff},1}(x, a, b)$, where $U^{\mathrm{eff},\sigma}(x, a, b)$ ($\sigma = 0$ or 1) is defined by

$$U^{\mathrm{eff},\sigma}(x, a, b) = \begin{cases} U(x, a, b) & (x \in \Omega_\sigma) \\ \infty & (x \in \Omega_{1-\sigma}) \end{cases} . \tag{7.10}$$

The work for the writing process, $W_{\mathbf{BCDA}}$, can therefore be given as the quasistatic work: Let us introduce the configurational free energies, $F(a, b; \Omega_0 \cup \Omega_1)$ and $F(a, b; \Omega_\sigma)$, corresponding to $U(x, a, b)$ and $U^{\mathrm{eff},\sigma}(x, a, b)$, respectively, by

$$e^{-F(a,b;\Omega_0\cup\Omega_1)/k_{\mathrm{B}}T} \equiv \int_{\Omega_0\cup\Omega_1} e^{-U(x,a,b)/k_{\mathrm{B}}T} dx, \tag{7.11}$$

$$\begin{aligned} e^{-F(a,b;\Omega_\sigma)/k_{\mathrm{B}}T} &\equiv \int_{\Omega_0\cup\Omega_1} e^{-U^{\mathrm{eff},\sigma}(x,a,b)/k_{\mathrm{B}}T} dx \\ &= \int_{\Omega_\sigma} e^{-U(x,a,b)/k_{\mathrm{B}}T} dx. \end{aligned} \tag{7.12}$$

Then the work of writing is expressed as follows with probability 1:[10]

$$W_{\mathbf{BCDA}} = F(a_{\mathrm{A}}, b_{\mathrm{A}}; \Omega_1) - F(a_{\mathrm{B}}, b_{\mathrm{B}}; \Omega_0 \cup \Omega_1), \tag{7.13}$$

Estimation of the Work of Erasure: $\mathcal{E}$

Let us calculate the work for the reverse operation of erasure, $W_{\mathbf{BA}}$, because it is intuitively simpler than the erasure process $W_{\mathbf{AB}}$, and because we know that these two works cancel with each other: $W_{\mathbf{AB}} = -W_{\mathbf{BA}}$. $W_{\mathbf{BA}}$ writes

[10] Hereafter a_{A}, etc., denotes the value of parameter a at the stage A, etc.

$$W_{\mathbf{BA}} = \int_{b_\mathrm{B}}^{b_\mathrm{A}} \frac{\partial U(x(t), a_\mathrm{A}, b(t))}{\partial b} db(t), \tag{7.14}$$

where we used $a_\mathrm{A} = a_\mathrm{B}$. By an analogy to Sect. 7.1.1.4, we raise quasistatically the barrier from $b = b_\mathrm{B}$ up to b^* such that $\tau_\mathrm{sys} \simeq \tau_\mathrm{op}$ for $b = b^*$. The corresponding work is

$$W_{\mathbf{B}*} = \int_{b_\mathrm{B}}^{b^*} \left[\int_{\Omega_0 \cup \Omega_1} \frac{\partial U(X, a_\mathrm{A}, b)}{\partial b} \mathcal{P}^\mathrm{eq}(X, a_\mathrm{A}, b) dX \right] db. \tag{7.15}$$

Then for $b^* < b \le b_\mathrm{A}$, we have $\tau_\mathrm{sys} \gg \tau_\mathrm{op}$. Suppose that x stays in a domain Ω_σ during this regime. The work of this part can be calculated as a quasistatic work with the effective potential energy, $U^{\mathrm{eff},\sigma}(x, a, b)$. The point is that *twice* the canonical distribution function ($\mathcal{P}^\mathrm{eq}(X, a, b) = e^{-U(X,a,b)/k_\mathrm{B}T}/Z$) should be used because the state is confined in Ω_σ:

$$\begin{aligned} W_{*\mathbf{A}} &= \int_{b^*}^{b_\mathrm{A}} \left[\int_{\Omega_0 \cup \Omega_1} \frac{\partial U^{\mathrm{eff},\sigma}(X, a_\mathrm{A}, b)}{\partial b} \, 2\mathcal{P}^\mathrm{eq}(X, a_\mathrm{A}, b) dX \right] db \\ &= \int_{b^*}^{b_\mathrm{A}} \left[\int_{\Omega_0 \cup \Omega_1} \frac{\partial U(X, a_\mathrm{A}, b)}{\partial b} \mathcal{P}^\mathrm{eq}(X, a_\mathrm{A}, b) dX \right] db. \end{aligned} \tag{7.16}$$

To go to the second line, we have used the symmetry of $U(X, a_\mathrm{A}, b)$ and of $\mathcal{P}^\mathrm{eq}(X, a_\mathrm{A}, b)$. Adding $W_{\mathbf{B}*}$ and $W_{*\mathbf{A}}$, we obtain the total work $W_{\mathbf{BA}}$

$$\begin{aligned} W_{\mathbf{BA}} &= F(a_\mathrm{A}, b_\mathrm{A}; \Omega_0 \cup \Omega_1) - F(a_\mathrm{B}, b_\mathrm{B}; \Omega_0 \cup \Omega_1) \\ &= -W_{\mathbf{AB}}. \end{aligned} \tag{7.17}$$

Total Work of the Overwriting Cycle, $\mathcal{E}+\mathcal{W}$

By adding $W_{\mathbf{AB}}$ and $W_{\mathbf{BCDA}}$, we have

$$\begin{aligned} W_{\mathbf{AB}} + W_{\mathbf{BCDA}} &= F(a_\mathrm{A}, b_\mathrm{A}; \Omega_1) - F(a_\mathrm{A}, b_\mathrm{A}; \Omega_0 \cup \Omega_1) \\ &= k_\mathrm{B}T \ln 2, \end{aligned} \tag{7.18}$$

because (7.11) and (7.12) give $e^{-F(a,b;\Omega_0\cup\Omega_1)/k_\mathrm{B}T} = 2\,e^{-F(a,b;\Omega_\sigma)/k_\mathrm{B}T}$. This is the main result of [2, 3]: Every operation of overwriting costs at least $k_\mathrm{B}T \ln 2$ of irreversible work. By the stochastic energetics the result holds for an individual process with the probability of one in the limit of slow operation.

The heat associated with this cycle has been analyzed using the stochastic energetics [10].[11] In the language of information, the memory σ specified through the

[11] [10] used the Bennett's definition of "copying" of memory. Since this definition does not complete a cycle, their results differ apparently from those in the text. However, these formulations are mathematically equivalent.

preceding writing process is lost irreversibly during the erasure process. The statistical entropy associated with the variable σ has been increased by $\ln 2$. The ensemble averaged irreversible work has been given in [11]. More recently [12] incorporated mechanical approach of the type of Jarzynski nonequilibrium work relation, and confirmed both analytically and numerically $k_B T \ln 2$ as the lower bound of the average irreversible work. [12] also analyzed the case where $U(0, a)/k_B T$ is moderately large.

7.1.2.3 Copying a Memory

What Does "To Know" Mean?

The "memory" is the state of a system ("bit memory"). The subject who "knows" the memory is, therefore, this system, not the external agent that controls the parameters a and b. For such ignorant external agent, the cycle of overwriting operation in Fig. 7.5 is optimal with the least average dissipation. Now we define "to know" (to acquire a knowledge) as the process by which a fixed memory of a system, called data bit [3], is correlated to the state of another system, called movable bit. In the ideal process "to know" the memory of a movable bit is rendered equal to the memory of the data bit with probability 1. We will say that the (memory of) data bit is *copied* to the (memory of) movable bit.

Cost-Free Copying Would Constitute a Perpetual Machine

A simple thought experiment shows that the external agent must pay a certain irreversible work to copy the data bit to the movable bit. Otherwise, the second law of thermodynamics would be violated.

Suppose that an external agent can copy the memory of a given data bit onto n ($\gg 1$) movable bits without cost. At this point, the external agent does not know the value σ of the copied bit. As the next step the external agent applies the reverse cycle of Fig. 7.5, i.e., A $\to$ D$\to$ C$\to$ B$\to$ A, to one of those movable bits. If $\sigma = 1$, the external agent will gain the work $\simeq k_B T \ln 2$ from the reverse cycle. If $\sigma = 0$, the work by the external agent is positive and much larger than $k_B T \ln 2$. The external agent thus knows the value of σ.[12] Then as the third step, the external agent applies to the remaining $(n - 1)$ copies the "correct" reverse cycle, either A $\to$ D$\to$ C$\to$ B$\to$ A of Fig. 7.5 if $\sigma = 1$, or its mirror image ($a \to -a$) if $\sigma = 0$, so that the external system gains work of $\simeq k_B T \ln 2$ from the $(n - 1)$ copies. This is possible because the external agent knows what σ is. In this way, the external agent could obtain a positive net work which increases with n. The whole operation would, therefore, constitute a perpetual machine of the second kind, which extracts a work from an isothermal environment.

[12] This operation need not be very efficient as long as $n \gg 1$.

The Cost of Copying is No Less Than $k_B T \ln 2$ Per Movable Bit

The operation of copying is a cycle: Every time a new data bit of unknown state σ is given, the external agent must erase the previous memory of a movable bit σ' to replace it with the value of σ. See Fig. 7.7. Therefore, the work of copying is derived in the same way as that of overwriting. We will show this below.

We will denote by x_0 and x the degrees of freedom of the data bit and the movable bit, respectively. To simplify the analysis, we will ignore the thermal fluctuation of x_0 (the left column in Fig. 7.7), although thermal fluctuations of x_0 within the domain Ω_σ will not change the conclusion. The potential energy for the movable bit, $U(x, a, b; \sigma)$, has two control parameters, a and b. The parameter b controls the barrier height of the double-well potential for x, and the parameter a controls the *distance* between this bit and the data bit.

Initially the two-bit memories are well isolated from each other, so that there is no interaction between the memories x_0 (or σ) and x. $U(x, a, b; \sigma)$ then takes a symmetric form (A in Fig. 7.7). At this position, the potential barrier for x is lowered through the parameter b (A$\rightarrow$B in Fig. 7.7). Then the movable bit is brought into interaction with the data bit. $U(x, a, b; \sigma)$ then becomes asymmetric in a σ-dependent manner (B$\rightarrow$C in Fig. 7.7).[13] At this position, the potential barrier for x is raised (C$\rightarrow$D in Fig. 7.7). Finally the movable bit is brought apart from the data bit (D$\rightarrow$A in Fig. 7.7).

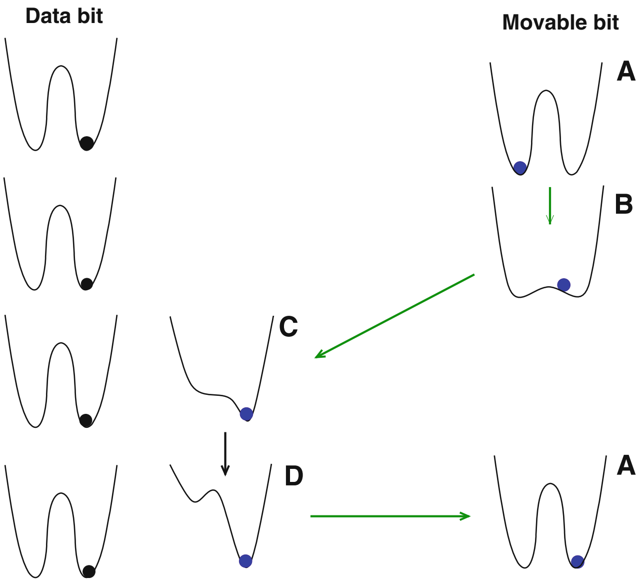

Fig. 7.7 The data bit (*left* column), and the energy involving movable bit *and* the interaction energy between the two bits, $U(x, a, b, \sigma)$ (*right*)

[13] We assume that the profile of $U(x, a, b; \sigma)$ and that of $U(x, a, b; 1-\sigma)$ are of the mirror images along the x-axis.

We realize that the complete cycle is essentially the same as the cycle of overwriting a bit memory shown in Fig. 7.5. The minimum cost of making copy of the data bit is, therefore, $k_B T \ln 2$. The only difference is that the asymmetry of the potential energy in the copying process is not determined by the control parameter a but is determined by the memory (σ) of the data bit. To conclude, we need the work to be no less than $k_B T \ln 2$ per movable bit. Therefore, we cannot make a perpetual machine.

7.1.3 * *Essentially Nonquasistatic Process Can Take Place upon the Relaxation from Non-Gibbs Ensembles of Fluctuations*

The second type of essentially nonquasistatic processes is related to the erasure process $\mathcal{E}$ in Sect. 7.1.2: The nonequilibrium state of the system is *irreversibly* equilibrated by an equilibrium environment.

7.1.3.1 Setup of the Problem and the Result

Let us consider the following cyclic operation of a system with two thermal environments. See Fig. 7.8(a) [13]. In (i) the system is thermalized with the thermal environment of temperature T_1. Then (ii) the system is slowly detached from the environment. (iii) Under complete isolation, the control parameter is slowly changed from a_1 to a_2. Then (iv) the system is slowly attached to the second thermal environment of temperature T_2. After the thermalization, the operations are retraced slowly back to the state (i). The value of a_2 is chosen so that, upon attachment to the environment of temperature T_2, no energy is exchanged *on the average* between the system and the new environment. The quantity of interest is the work needed to change the parameter a:

$$W = \int_{a_1:(ii)\to(iii)}^{a_2} \frac{\partial H(x(t), p(t); a(t))}{\partial a} \circ da(t) + \int_{a_2:(iii)\to(ii)}^{a_1} \frac{\partial H(x(t), p(t); a(t))}{\partial a} \circ da(t),$$

where $H(x, p; a)$ is the system's energy as a function of position x and the momentum p. We ignore the work of detachment and attachment with the thermal environments, since they were shown to be reducible as small as needed.

If the system is macroscopic, the choice of a_2 amounts to equalizing the system's temperature to T_2 before the contact with the second heat bath. Under this condition, the process is reversible in the limit of quasistatic adiabatic operation, and the work W is 0.[14]

For the mesoscopic system, several aspects are different from the macroscopic case:

1. The work W fluctuates from one realization to the other, however, slowly the operations are done.

[14] Unlike the Carnot cycle, the parameter a is not changed under isothermal condition.

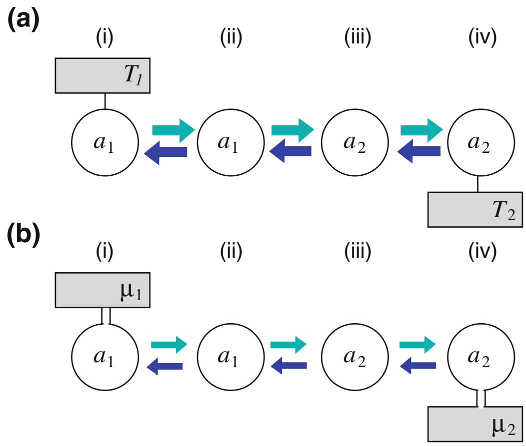

Fig. 7.8 A protocol including the detachment and attachment with heat baths (**a**) or with a particle reservoirs (**b**). The numbers, (*i*), etc., refer to those in the text. The system's parameter a is changed in the processes (*ii*)$\rightleftharpoons$(*iii*), where the system is isolated from these environments. (The figure is modified from Fig. 1 of [13])

2. The ensemble average of W is nonnegative even in the limit of slow operations.[15] Only for special class of systems (see below) the average work $\langle W \rangle$ can tend to 0 in the limit of slow operations.

A similar problem can be set up for the open system. See Fig. 7.8(b). Here the operations of detachment–attachment are done with the particle environments of different chemical potentials μ_1 and μ_2. And the operation of (ii)$\rightleftharpoons$(iii) is quasistatic isothermal process without particle exchange. The value of a_2 is chosen so that, upon the making contact with the environment of chemical potential μ_2, no particles is exchanged *on the average* between the system and the new environment. Again the average work $\langle W \rangle$ is positive, except for the special systems where $\langle W \rangle$ tends to 0.

7.1.3.2 Analysis of the Operations

Below we will analyze the elementary physical processes included in this intriguing cycle. As for the proof of the above statements, interested readers may consult [13, 14]. The paper uses the Kullback–Leibler distance defined for the ensemble of processes.

Slow Detachment from an Environment

This is essentially a nonquasistatic process. Although the associated work can be made negligibly small, the system's state becomes constrained after this operation:

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[15] Roughly speaking, the system's energy at the end of return operation, (iii)→(ii), is on average higher than the initial thermalized state. Therefore, during the operation (ii)→(i) the heat $\langle(-Q)\rangle = \langle W \rangle$ is dissipated to the thermal environment.

in Fig. 7.8(a) the system's energy E is constrained to obey $dE = dW$ because the heat exchange is blocked, and in Fig. 7.8(b) the number of particles n is fixed. The work to change the parameter a depends on these fixed values. Therefore, W fluctuates from one realization to the other, however, slowly the operations are done.

Just after the detachment the distributions of E in Fig. 7.8(a) or n in Fig. 7.8(b) obey, respectively, the canonical or grand canonical distributions if the detachment is slow enough. In fact, the end of the detaching process (either (i)→(ii) or (iv)→(iii)) is very unpredictable for the external system. Therefore, the values of E or n at this last moment will be found with the probability proportional to their residence–time distribution. If the detaching process from an environment is quasistatic except at the last moment, then this distribution is the Gibbs statistical weight at the temperature or chemical potential of the (detaching) environment.

Adiabatic Process or Process Without Particle Exchange

The operations between (ii) and (iii) are deterministic in the energy E for Fig. 7.8(a) and in the particle number n for Fig. 7.8(b). For (a) the so-called adiabatic invariant remains constant during this process, while for (b) it is n that is invariant. In the course of this process, the probability distributions of these quantities are transformed accordingly from the initial Gibbs statistical weight to another distributions which depend on a.

At the end of these operations, distributions of E or n are generally different from the Gibbs statistical weight for the system at any T or μ, respectively. The exceptions are those systems in which (i) E or n take only two quantized values or (ii) the potential energy $U(x, a)$ takes the form of $k(a)|x|^{\alpha}$ with α a constant.[16] Generally, the system's E or n are brought to non-Gibbs distribution.

Attachment with a New Equilibrium Environment

This operation renders the above mentioned non-Gibbs distributions of energy E or number of particles n to the Gibbs statistical weight appropriate for the new environment. This process is irreversible.

We could avoid this irreversibility if there is a macroscopic and reversible operation that transforms the non-Gibbs distribution to a Gibbs distribution *before* the operation of attachment. Except for the special systems [15] there is no such protocol. The key issue is that it seems impossible to select reversibly those systems which have a prescribed energy.[17] Let us call such hypothetical reversible cycle *selecting operation*.

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[16] For quantum system, this condition leads to the relations among the energy levels, $E_\nu(a') - E_0(a') = \phi(a, a')[E_\nu(a) - E_0(a)]$, where $\phi(a, a')$ is a given function. For the open system the list of exceptional cases is not exhaustive.

[17] A similar argument should be made for the open system.

The argument against this operation is as follows [16]. There is a concrete reversible operation to extract positive work from an initially microcanonical ensemble (i.e., the systems having the same energy).[18] Let us call this operation the *work-extracting operation*. Now this operation is incompatible with the existence of the selecting operation. In fact, if the both operations could be done reversibly, we could (i) detach a system from a thermal environment, (ii) use the selecting operation to check if the system has a prescribed energy, then (iii) if yes, apply the work-extracting operation to extract a work, or if otherwise, do nothing, and finally (iv) reattach the system to the original thermal environment. In this way we could constitute a perpetual machine of the second kind.

In conclusion, at least to our present understanding, the cyclic process in Fig. 7.8 is generally unavoidably irreversible because of an essentially nonquasistatic process of attachment to the environment.

7.2 Detection and Control Under Fluctuations

*7.2.1 * Two Types of Error-Free and Unbiased Detection Under Fluctuation are Possible*

Detection is a process that correlates the exterior of a system to the system's state. We focus on the detection of a particle coming randomly from outside to the system. Signal particles undergo random motion in the environment. When one of them happens to arrive at the detection site of a sensor, and if the sensor establishes a correlation with this event, the sensor acquires a signal as information.

Examples of signal detection are found everywhere. In biology, some motor proteins work at very good efficiency of free-energy conversion.[19] Those motor proteins must not spend a lot of energy source in the detection of the fuel particle (e.g., ATP) or of the object of work (e.g., actin filament). Some gene regulations are very precise, while they use highly irreversible reactions with kinase or phosphatase, etc. In optics, a CCD camera uses photoelectric transitions to detect light signals, and its signal-to-noise ratio depends on the temperature.

Now, questions are

(1) Is it possible to realize a mesoscopic single-particle sensor which works correctly without bias or errors under thermal fluctuations?
(2) If it is possible, what aspects of the usual sensors in the macroscopic world should be abandoned?

These are the main themes of this section.

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[18] For the canonical ensemble, the similar operation immediately contradicts the second law of thermodynamics. But it is possible for microcanonical ensemble.

[19] Some claims that the motor proteins like F1ATPase are working at about 100% efficiency.

7.2.1.1 Half-Sensors

Let us distinguish the two notions about the detection, which we call IN/OUT and ON/OFF. A signal particle is said to be IN if it is present at the "detection site" of the sensor, and otherwise it is OUT. The sensor is assumed to take two internal states ON and OFF. The ON [OFF] states of the sensor are designed to be positively correlated to the signal particle's state, IN [OUT], respectively. IN and OUT are the objective fact about the presence or absence of the particle, while ON and OFF are the perception by the sensor about the particle.

Figure 7.9(a) shows those correlations in the ordinary sensor. The two shaded zones are prohibited to occur and these constraints allow one-to-one correspondence between the sensor's states and the arrival of signal particles.

In the mesoscopic scale, the unbiased and error-free detection is still possible if we sacrifice one of these two prohibition zones. We define two types of half-sensors by the tables Fig. 7.9b, c. In response to the particle's state IN/OUT, these sensors are multivalued functions in the range ON/OFF. The "half-absence sensor" can have the state OFF only when the particle is OUT. Thus if the sensor thinks that the particle is OFF, the signal particle is surely OUT without bias or errors. But this "absence" sensor can miss the particle's absence OUT by thinking it be IN. The "half-presence sensor" works completely complementary manner to the "half-absence sensor."

The half-sensors can be designed to work reversibly (see below).[20] The possibility of the usual sensor (Fig. 7.9a) on the mesoscopic scale is not known. A usual sensor can be made as the composite of Fig. 7.9b, c. This corresponds to the product of two Boolean variables. Since the product of two Boolean variables is an irreversible operation, the function of such composite sensor might need some free-energy resource (see [17]).

The utilities of the two types of half-sensors are different. For example, if the signal particle is "toxic" for a system, the system can use the OFF sign of the half-absence sensor. This OFF signal is analogous to the regulation of gene transcription by a repressor protein [18], since the transcription is surely prohibited

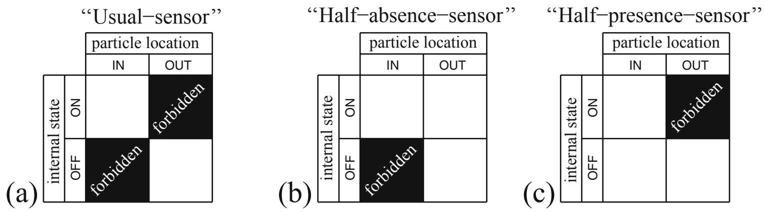

Fig. 7.9 The functions of the usual sensor (**a**) and the two kinds of half-sensors (**b**) and (**c**). The *black squares* indicate the forbidden situations

[20] Therefore, the half-sensors are different from "to know," which is irreversible and essentially nonquasistatic process.

by the repressor protein bound to the operator site on the DNA. By contrast, if the particle is the "food" for a system, it can use the ON sign of the half-presence sensor. This is analogous to the activation of the repressor protein, since the activation of the repressor surely requires the signal particle. Also the uptake of ATP molecule by a molecular motor will be analogous to the half-presence sensor.

7.2.1.2 Construction Principles of the Half-Sensors

On the scale of thermal fluctuations, the only way to avoid the errors of detection due to thermal noises is to use the high (free) energies of interaction with respect to $k_B T$. At the same time, the total free energy of the sensor *plus* the signal particle should be unbiased upon detection. In order to meet these two conditions at the same time, there are two principal ways. The half-absence sensor uses the short-range steric (repulsive) interaction, while the half-presence sensor uses the compensation between strong attraction and strong restoring force. Below we use a 1D representation for the particle's position x and use a sensor's state variable a as the second coordinate.

Interaction Potential of the Half-Absence Sensor

Steric interaction between two bodies excludes the coexistence of these two at the same position. For example, if a coffee cup and a coffee pot cannot be put on a saucer at the same time, the coffee cup on the tray implies the absence of the coffee pot. The half-absence sensor uses this principle.

We assume that the position of a signal particle, x, can move in a half space $0 \le x < \infty$ and that $x = 0$ corresponds to the detection site (Fig. 7.10 *Left*). The state variable of the sensor, a, represents the leftmost point of a movable object (thick bars in Fig. 7.10 *Left*). a is allowed to move in the region of $-1 \le a \le 0$. A steric interaction is assumed between this object and the particle (thick dot). Then the signal particle is surely in the OUT state whenever the movable object is in the OFF state.[21] By construction, the total energy of the sensor plus the signal particle is constant over the allowed region on the reaction plane (shaded in Fig. 7.10 *Right*).

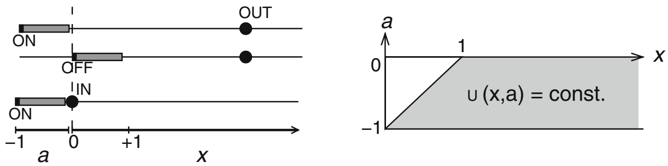

Fig. 7.10 *Left:* Schematic representation of the half-absence sensor. The *thick bar* (a: the *leftmost* position) and the *thick dot* (x) repel with each other by steric repulsive interaction. *Right:* On the (x, a)-plane the shadowed region is accessible without bias

[21] The total energy of the ligand–sensor system, $U(x, a)$, is written as $U(x, a) = U_0$ for $x \ge a+1$ and $U(x, a) = \infty$ otherwise. The sensor's states are assigned as OFF for $a \ge -1+\delta$ and as ON for $-1 \le a < -1+\delta$, respectively, with a small $\delta > 0$.

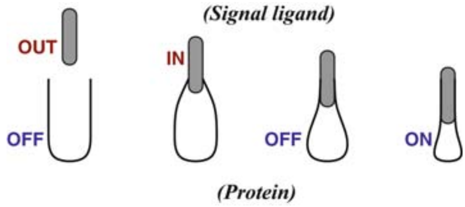

Fig. 7.11 The notion of *induced fit*. As the signal ligand is bound progressively by the protein, the protein deforms accordingly

Interaction Potential of the Half-Presence Sensor

The notion of the compensation of energies has long been discussed in biology [19]. Suppose that a signal ligand (particle) can gradually make strong attractive interactions with the sensor protein. Suppose also that this interaction causes the sensor to deform with a large free-energy cost.[22] See Fig. 7.11. Koshland called this deformation *induced fit* [19]. Now if the gain of the attractive interaction energy is almost compensated by the cost of sensor's deformation up to $\sim k_{\mathrm{B}}T$, the deformation of the sensor surely indicates the presence of the ligand particle without bias. In this case the induced fit realizes the half-presence sensor with a being the sensor's deformation.

Figure 7.12 *Left* shows schematically the relation between the signal particle x and the sensor's state a. If the signal particle is present ($x \sim 0$), the short-range attraction between x and a comes into action while the displacement of a from the resting position $a = -1$ costs deformation energy. As a result of the energy compensation, there appears an unbiased corridor of total free energy (shadowed region in Fig. 7.12 *Right*).[23] More precisely, the sensor's state is ON for $a \geq -1+\delta$

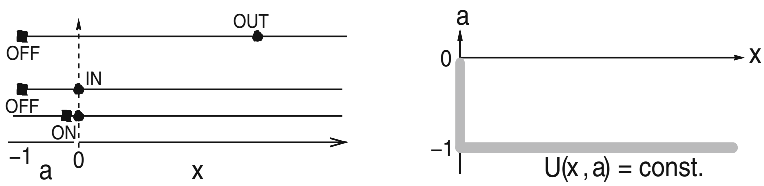

Fig. 7.12 *Left:* Schematic representation of the half-presence sensor. The *filled square* (a: sensor "tip") and the *thick dot* (x) attract each other for $|x-a| \leq 1$, while the displacement in the $a > -1$ region provokes a restoring force. *Right:* On the (x, a)-plane the shadowed region is accessible without bias

[22] The cost may be either energetic such as of mechanical deformations or entropic such as of folding. The detail of the process may contain the aforementioned jump-and-catch process.

[23] The total energy of the ligand–sensor system, $U(x, a)$, is the sum of short-range strong attractive interaction energy, $-M\phi(a-x)$ ($M \gg k_{\mathrm{B}}T$), between the ligand particle and the sensor "tip" and also strong restoring potential $M\phi(a)$. Here $\phi(z)$ ($-\infty < z \leq 0$) is $\phi(z) = 0$ for $z \leq -1$ and monotonically increasing from $\phi(-1) = 0$ to $\phi(0) = 1$.

and OFF for $-1 \leq a < -1 + \delta$, respectively, where δ is determined as the position where the deformation energy exceeds some $k_B T$.[24]

Remarks

Discretization of state and the half-presence sensor: In looking at Fig. 7.12, one might wonder if the sensor is actually bijective, like Fig. 7.9a. However, the discretization of the sensor's state and the particle's position requires the *gray* zone of (IN, OFF), because the judgement of OFF→ON requires the presence of particle (IN) so that an energy more than $k_B T$ is exchanged between the attracting potential and the restoring potential.

Timescale of sensing: The diffusion of small signal particles can be too rapid for the sensor to follow adiabatically.[25] This is also the reason to distinguish the particle's position and the sensor's state.

Relation between the half-absence sensor and half-presence sensor: The half-presence sensor is, in some sense, on the basis of the half-absence sensor. In fact, for the latter sensor, the object that interacts sterically with the signal particle (the thick bars in Fig. 7.10 *Left*) must be sensed elsewhere.

Signal sensing must have a consequence: An isolated sensor serves nothing. The state of the sensor must be coupled to its "downstream" mechanisms, e.g., by accelerating an enzyme reaction, modifying the access of another molecule to the system, etc. Through this coupling, the sensing process can become biased and irreversible.[26]

Technical Remarks

Reaction coordinate of the presence sensor: In Fig. 7.12 *right*, the detection of the particle occurs through an unbiased corridor corresponding to the unbiased valley of the total potential energy. Therefore, a single reaction coordinate

$$\tilde{x} \equiv x - a \qquad (0 \leq \tilde{x} < \infty) \tag{7.19}$$

can parametrize this pathway. The inversion to the values of x and a is given by

$$x(\tilde{x}) = \max(\tilde{x} - 1, 0), \quad a(\tilde{x}) = -\min(\tilde{x}, 1). \tag{7.20}$$

By definition $U(x(\tilde{x}), a(\tilde{x}))$ is constant.

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[24] i.e., $M\phi(-1 + \delta) \sim k_B T$. The consistency of these assignments with the above definition can be verified by scrutinizing the graphs of $M\{\phi(a) - \phi(a - x)\}$ vs. a for various values of x.

[25] Biological sensor may be designed to avoid this.

[26] Sect. 7.2.1.4 is an example.

Fig. 7.13 *Left*: the (x, a) pathway between the right environment $(x > 0)$ and the *left* environment $(x < 0)$ through the detection site $x = 0$. *Right*: extended reaction coordinate $\tilde{x}$, where the a coordinate is duplicated to $-1 \le \tilde{x} \le 1$

Extension of the reaction coordinate: If a half-presence sensor is accessible from two-particle reservoirs, the two access routes can be distinguished as $x > 0$ and $x < 0$. See Fig. 7.13 *Left*. In that case the reaction coordinate $\tilde{x}$ $(-\infty < \tilde{x} < \infty)$ may represent x and a by

$$x = \frac{\tilde{x}}{|\tilde{x}|} \max(|\tilde{x}| - 1, 0), \quad a = -\min(|\tilde{x}|, 1). \tag{7.21}$$

See Fig. 7.13 *Right*. For $|\tilde{x}| \le 1$, the pair of points $\{+\tilde{x}, -\tilde{x}\}$ should be identified as a single physical state, $(x(\tilde{x}), a(\tilde{x}))$. This technical trick is convenient for discussing the coupled transport in Chap. 8.

7.2.1.3 Balance of Forces in the Half-Presence Sensor

Apart from the energetic compensation, the mechanical force balance should hold when a half-presence sensor detects a particle. Figure 7.14 illustrates how the forces act among different elements while the sensor undergoes the transition, OFF→ON.

In this figure, the signal particle at the detection site $(x = 0)$ feels the attractive force from the sensor tip ("movable portion of the sensor"). The particle cannot enter into the $x < 0$ region because the "main body of the sensor" pushes back the particle through the steric repulsion. The sensor tip feels both the attractive force from the particle and the restoring force from the main body. These two forces should be

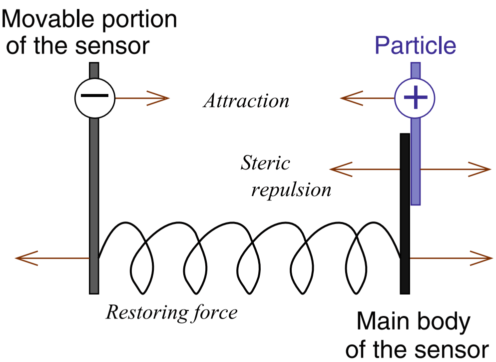

Fig. 7.14 The balance of forces among the three constituents of the half-presence sensor

balanced in an unbiased sensor. The main body of the sensor is pushed to the left by the particle, while it is pushed to the right by the restoring force of the sensor tip.

In terms of the flux of momentum in the x direction, Fig. 7.14 represents a permanent circulation of the momentum [20].[27] A similar mechanical analysis can be done for the induced fit in Fig. 7.11.

7.2.1.4 Functions of Coupled Sensors

If two half-sensors are energetically coupled, their individual functions as sensors are modified, on the one hand, but they can acquire various functions as a composite system. Two examples are discussed below.

Suppose that a composite system has two half-presence sensors, sensor 1 and sensor 2 with (x_1, a_1) and (x_2, a_2) being the pairs of signal particle position and state variable. As the coupling energy between these half-sensors, we take two examples of the quadratic form, $\Lambda(a_1 - a_2)^2$ or $\Lambda(a_1 + a_2 + 1)^2$, where $\Lambda > 0$ is a constant. In the biophysics of proteins, the coupling among different degrees of freedom in a protein is called allosteric coupling, and the effects due to this coupling is called *allosteric effects*. See, for example [21].

Case of $\Lambda(a_1 - a_2)^2$: allosteric transition [22, 23]

The coupling energy favors a synchronized response of the two sensors with $a_1 \simeq a_2$. See Fig. 7.15 *Top*. If the signal particles in the environment visit at random the detection sites, $x_1 = 0$ and $x_2 = 0$, the cooperative transition of the states (a_1, a_2) from $(\mathsf{OFF}_1,\mathsf{OFF}_2)$ to $(\mathsf{ON}_1,\mathsf{ON}_2)$ is likely to occur when the signal particles for both sensors are in the ON positions, $x_1 \simeq x_2 \simeq 0$. Especially when the two half-sensors detect the same species of particles, the probability of cooperative transition depends quadratically on the density of signal particles. Such nonlinear transitions are called *allosteric transition* Fig. 7.16 *Left* represents the process of allosteric transition on the plane of reaction coordinates, $(\tilde{x}_1, \tilde{x}_2)$. [22, 23]. [28]

Case of $\Lambda(a_1 + a_2 + 1)^2$: exchange of binding[5]

The coupling energy $\Lambda(a_1+a_2+1)^2$ takes the minimum value 0 when $a_1+a_2 = -1$. If $\Lambda \gg k_B T$, this system is, therefore, no longer unbiased sensor, but it rather likes to fill particles in at least one of the half-sensors. As we will see below, this system functions as the *exchange of binding* between two allosteric sites.

Suppose that, at present, the system binds only one particle. The state of the composite system is, therefore, $(\mathsf{OFF}_1,\mathsf{ON}_2)$ or $(\mathsf{OFF}_1,\mathsf{ON}_2)$. This state will remain

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[27] The $+x$-oriented momentum flows toward $+x$ along the attractive force and toward $-x$ along the repulsive (restoring) force.

[28] A similar phenomenon has been observed for the binding of ATP-activated kinesin molecules to a microtubule, called the *cooperative binding*, [24].

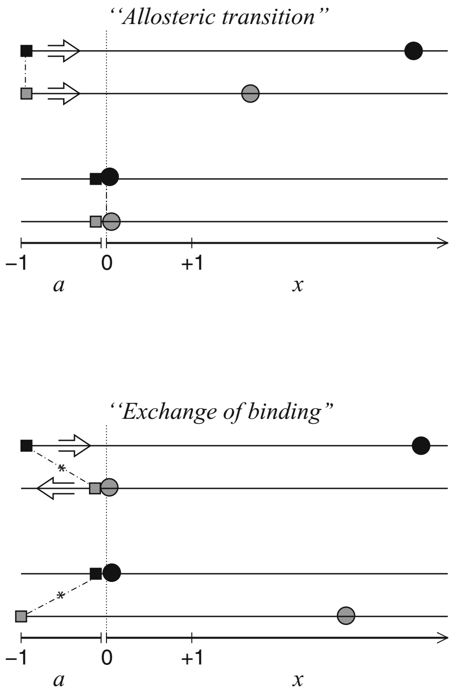

Fig. 7.15 *Top*: Allosteric transition by the coupling $\Lambda(a_1 - a_2)^2$. *Bottom*: Exchange of binding by the coupling $\Lambda(a_1 + a_2 + 1)^2$. For the symbols, see the caption of Fig. 7.12

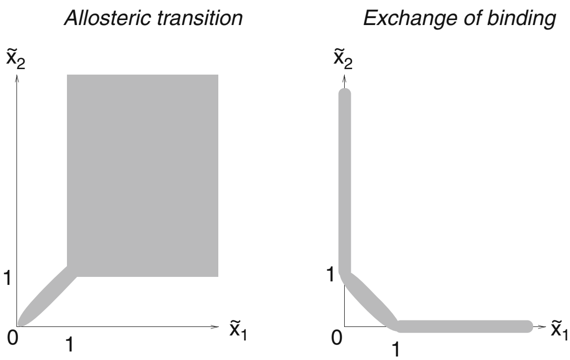

Fig. 7.16 *Left*: Allosteric transition by the coupling, $\Lambda(a_1 - a_2)^2$. *Right*: Exchange of binding by the coupling, $\Lambda(a_1 + a_2 + 1)^2$. $(\tilde{x}_1, \tilde{x}_2)$ are the reaction coordinates (7.19) for the two half-presence sensors. The shaded region is the region of a constant energy

stable until the second particle arrives at the half-sensor in the unoccupied (OFF) state. Once the two half-sensors bind their signal particles, the state variables (a_1, a_2) can diffuse along the line of $a_1 + a_2 = -1$. When (a_1, a_2) arrive either at $a_1 = -1$ or $a_2 = -1$, it is possible that one of the particles leaves the detection site. See Fig. 7.15 *Bottom*.[29] As a result, the switch between (OFF_1,ON_2) and (OFF_1,ON_2) can be realized without passing the (OFF_1,OFF_2) state. Figure 7.16 *Right* represents the process of exchange of binding on the plane of reaction coordinates, $(\tilde{x}_1, \tilde{x}_2)$. If there is a bias between $(a_1, a_2) = (-1, 0)$ and $(0, -1)$, the arrival of the particle with higher "affinity" can expel the previously bound particle by the allosteric effect.

7.2.2 * The Gates to Control Particle's Access Can be Made Using Adjustable Potential Barriers

Definition of Gate

Suppose that a detection site of a half-presence sensor is accessible both from the left-particle environment ($x < 0$) and from the right-particle environment ($x > 0$). The gate for these environments is a mechanism such that the signal particles can get access to the detection site exclusively from one of these environments. In the extended reaction coordinate, $\tilde{x}$ (see Fig. 7.13 and (7.21)), the gate implies a blockade either between $(-\infty, -1)$ and $[-1, 1]$ or between $[-1, 1]$ and $(1, \infty)$.

Gate Made by the Potential Energy Barriers

We introduce potential barriers localized around $x = \pm\epsilon$ with a small width $2\epsilon > 0$. In the extended reaction coordinate, the barriers are made around $\tilde{x} = \pm(1 + \epsilon)$, see Fig. 7.17. When only the left barrier is established with the height of $M \gg k_{\mathrm{B}}T$ (Fig. 7.17 *Top*), the access of the particles from the left environment is blocked. The situation is inverted when only the right barrier is established (Fig. 7.17 *Bottom*). The gate is realized by adjusting the heights of these two barriers so that at any time at least one of the barriers is high enough compared with $k_{\mathrm{B}}T$. The irreversible work to raise or lower the potential barriers is negligible for small ϵ (see Sect. 7.1.1.4). The reaction force from the particles against the operation of the barriers is negligible because of the steep gradient of the barrier profile.

Margins of Operation

A small positive number ϵ has been introduced to represent the fact that the potential barriers should be located outside but close to the detection sites. Although the irreversible work of operating the gate can be made negligible, this ϵ, as well as

[29] This is the first passage time (FPT) problem. See Sects. 1.3.3.3.

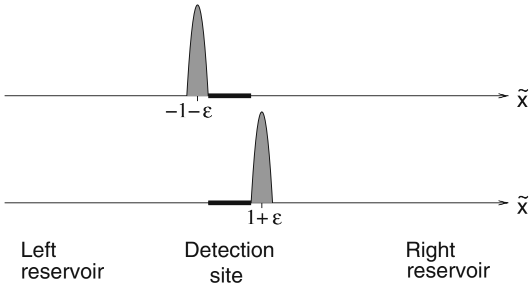

Fig. 7.17 Potential energy barriers of the gate for particles. $\tilde{x}$ is the extended reaction coordinate for the particle. *(Top)* Particles are accessible only from the *right*-particle environment. *(Bottom)* Particles are accessible only from the *left*-particle environment

the small δ introduced in the model of sensors (Sect. 7.2.1), constitute the source of small "leakage" when we construct free-energy transducers.

When we discretize the model in the form of the reaction networks, neglecting this marginal effect can sometimes lead to unphysical results. Especially caution must be maintained when one claims a strictly tight coupling or a 100% efficiency for a model of autonomous free-energy transducer.

7.3 Discussion

7.3.1 Control of Open System Has Both Common and Distinguished Features with Respect to the Control of Closed System

7.3.1.1 Parallelism with the Control of Closed System

The following list summarizes how the results of closed system can be generalized for the open system.

Quasistatic process: Quasistatic work under a fixed chemical potential μ of particle environment obeys the law, $W = \Delta J$, for each realization of process (Sect. 5.2.1.4).

Nonnegativity of the average irreversible work: When the external parameter is changed from a_{i} to a_{f} nonquasistatically, the average irreversible work $\langle W_{\mathrm{irr.}}\rangle \equiv \langle W\rangle - \Delta J$ is nonnegative. The nonequilibrium work relation applied to the entire system (see (5.59)[25]), $\langle e^{-W+\Delta F_{\mathrm{tot}}}\rangle = 1$, can be reduced to the equality for the open system,

$$\langle e^{-W+\Delta J}\rangle = 1, \tag{7.22}$$

where (5.18) is used.[30] By the Jensen inequality, $\langle e^{-x}\rangle \geq e^{-\langle x\rangle}$, we have

$$\langle W\rangle \geq \Delta J. \tag{7.23}$$

[30] The average $\langle\cdot\rangle$ is taken over all realizations starting from a pertinent equilibrium ensemble.

Complementarity relation: The average irreversible work $\langle W_{\text{irr.}} \rangle$ and the time spent for the process, Δt, satisfy the relation parallel to (5.36) [26]:

$$\langle W_{\text{irr.}} \rangle \, \Delta t \geq S(a_\mathrm{i}, a_\mathrm{f}) \qquad (\Delta t \to \infty), \tag{7.24}$$

where $S(a_\mathrm{i}, a_\mathrm{f})$ is independent of the (rescaled) protocol $\tilde{a}(s)$ between a_i and a_f.

Attachment/detachment with/from particle environment: The adiabatic process of the closed system corresponds to the closed isothermal process. The attachment with and detachment from the particle environment are realized by the raising and the lowering of the potential barrier (see Sect. 7.1.1.3). These processes are inevitably nonquasistatic (see Sect. 7.1.1.2).

Irreversible relaxation of probability distribution: See Fig. 7.8b.

"Carnot cycle": "Carnot cycle" for open systems extract work from the transport of particles between the particle environments of different chemical potentials μ_H and μ_L. See Fig. 7.18 below. In the next chapter we will present a concrete model of this cycle. The maximum available work is $(\mu_\mathrm{H} - \mu_\mathrm{L}) \times \langle n \rangle$, where $\langle n \rangle$ is the number of transfered particles.

7.3.1.2 Distinguishing Features of Open System

Basic facts are

(i) Unlike absolute temperature, chemical potential has a no absolute zero and admits indefinitely negative values.
(ii) Unlike a heat engine, the transferred particles of a particle engine do not necessarily carry energy.

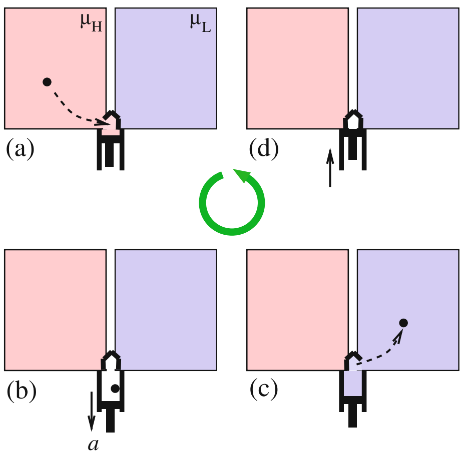

Fig. 7.18 A "Carnot cycle" to extract work. The particle (*thick dot*) enters from a dense particle environment of the chemical potential μ_H (**a**). The piston is pulled while the system is closed (**b**). The particle exits to the dilute particle environment of the chemical potential μ_H (**c**). The piston is pushed while the system is closed (**d**). If the dilute environment is vacuum ($\mu_\mathrm{L} = -\infty$), the infinite work can be extracted in principle

In regard to (i) a vacuum environment has the chemical potential of $\mu = -\infty$. Then thermodynamics implies that the maximum available work is positive infinity. By the fact (ii), the energy for this infinite work should be provided by the thermal environment, not by the transferred particles. See Fig. 7.18 for illustration. In this figure the open system consists of a cylinder furnished with a door and a movable piston. The starting point is a cylinder with the door being open to the particle environment of chemical potential $\mu_{\rm H}$. After a while the door is closed and the cylinder volume V is dilated indefinitely. At this point the cylinder contains particle(s) with a finite probability. The extracted work $(-W)$ can, therefore, be arbitrarily large by a large dilatation.[31] The flow of energy is from the thermal environment to the piston via the kinetic energy of the particles. After this dilation, the door is again opened, but now to the second particle environment of chemical potential $\mu_{\rm L}$, which has no particle ($\mu_{\rm L} = -\infty$). We wait patiently at this stage: Since the particles can only go out from the cylinder but cannot enter nor reenter, the cylinder becomes empty.[32] After closing the door, the next cycle restarts.

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[31] For the ideal gas particle, the quasistatic isothermal work $(-W)$ is $(-W) \propto k_{\rm B}T \ln(V_{\rm f}/V_{\rm i})$, with $p \propto k_{\rm B}T/V$ the pressure and $V_{\rm i}$ [$V_{\rm f}$] are the initial and final values of volume, respectively.

[32] It may take a long time $\propto V_{\rm f}$.

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