

Chapter 2. Principles of Physical Statistics

In this chapter we discuss such basic notions of statistical physics including probability, statistical ensembles, probability density, and density matrix. Then we use the basic statistical hypothesis, as formulated for the microcanonical ensemble, to define entropy. After that we use the notion of canonical ensemble to derive the Gibbs distribution (which is the central point of statistics). After that we discuss the partition function and the grand canonical ensemble.

2.1. Statistical Ensembles, Probability, and Probability Density

As has been already discussed in the beginning of Chapter 1, statistical physics deals with systems in conditions when either the initial conditions are not fully known or the laws of motion as such (as in the case of quantum mechanics) cannot give definite results of measurements. The main mathematical tool for the analysis of such systems is the probability theory, so that we will start with a very brief summary of its basic concepts. Let us carry out independent N experiments with apparently similarly prepared systems.¹ (The standard, and very convenient example is tossing a coin.) In the conditions of incomplete knowledge, the systems are internally still different, so that experiments may give different results (in the case of tossing a coin, heads or tails). Such a collection of experiments is called a *statistical ensemble*.

Let us start with the simplest case when the experiment may have M different outcomes, and count the number of experiments, N_1, N_2, \dots, N_M giving the corresponding results, so that

$$\sum_{j=1}^M N_j = N. \quad (1)$$

The *probability* of each outcome is then defined as

$$w_j = \lim_{N \rightarrow \infty} \frac{N_j}{N}. \quad (2)$$

Though the definition is so close to our everyday experience that it is almost self-evident, two remarks may still be relevant. First, it is evident from the definition that probabilities w_j depend on the exact statistical ensemble they are defined for. (As an exaggerated example, for the ensemble of coins before tossing, the probability of heads or tails is $1/2$. However, if we define an ensemble of all coins already on the floor with heads up, the probability of finding coins with tails up in this ensemble is zero.)

Second, the reference to infinite N in Eq. (2) does not strip the notion of probability from its practical relevance. Indeed, it may be proved (see Ch. 6) that at finite but large enough N the numbers N_j are in most cases relatively close to their “expectation values”

$$\langle N_j \rangle \equiv w_j N. \quad (3)$$

¹ Note that this does not necessarily require having N physical systems. All conclusions of the probability theory are also valid for N experiments with the same system, provided that the experiments are independent, i.e. that an outcome of past experiments do not affect those of the experiments to follow.

Let us now list the properties of probabilities, which we will immediately need. (We will keep coming back to the probability theory as we need more of its results.) First, dividing Eq. (1) by N and following the limit $N \rightarrow \infty$, we get the *normalization condition*

$$\sum_{j=1}^M w_j = 1. \quad (4)$$

Next, if we have an additive function of the experiment results

$$F = \frac{1}{N} \sum_{j=1}^M N_j F_j, \quad (5)$$

where F_j are some known (“deterministic”) coefficients, then we can define the *average* (or *expectation*)² value of the function as²

$$\langle F \rangle = \frac{1}{N} \sum_{j=1}^M \langle N_j \rangle F_j, \quad (6)$$

So that using Eq. (3) we get

$$\langle F \rangle = \sum_{j=1}^M w_j F_j. \quad (7)$$

In classical systems, the spectrum of possible experimental outcomes is frequently continuous. (Think about the positions of marks left by bullets fired in a target from a far.) The above formulas may be readily generalized to this case; let us start from the simplest case when all different outcomes may be described by one continuous variable x which replaces the discrete index j in Eqs. (1)-(7). The basic relation for this case is the evident fact that the probability dw of having the outcome corresponding to an infinitesimal interval dx (in our example, of having a bullet mark within that interval) is proportional to the magnitude of that interval:

$$dw(x) = \rho(x)dx. \quad (8)$$

The factor $\rho(x)$, which does not depend on dx , is called the *probability density*. Now all the above formulas may be re-cast by replacing the probability for the probability density, and the summation over j by integration over x . In particular, instead of Eq. (4) we now have

$$\int \rho(x)dx = 1, \quad (9)$$

Where the integration limits should embrace all the possible values of the experimental result x . Similarly, instead of a function F defined by Eq. (5) it is natural to expect that in the continuous case the important functions are functions of x : $f = f(x)$. Then instead of Eq. (7) we get the expectation value

² The averaging over the statistical ensemble, which is discussed here, from averaging over time. While for some systems (called ergodic) these two averages give similar results, in many important cases they are very much different. This is why we will use different signs for the statistical averaging $\langle F \rangle$ and time averaging \bar{F} .

$$\langle f \rangle = \int w(x) f(x) dx. \quad (10)$$

Now it is easy to generalize these formulas to the case of more variables. For the example of bullets shot into a plane target, x should be replaced by two coordinates (say, x and y) defining the position of the bullet mark on that plane. In this case the probability density ρ becomes a function of two variables, x and y , and the 1D integrals in Eqs. (9) and (10) should be replaced by 2D integrals over the target area.

Closer to the traditional tasks of statistical mechanics, a system of N classical particles (without holonomic constraints) is described by $6N$ variables, e.g., $3N$ Cartesian components q of the particle radius-vectors, and $3N$ components p of N momenta vectors. As a result, the probability density is now a function of $6N$ variables, and the expectation value of a typical function of these coordinates is a $6N$ -dimensional integral

$$\langle f \rangle = \int w(q_1, q_2, \dots, q_{3N}; p_1, p_2, \dots, p_{3N}) f(q_1, q_2, \dots, q_{3N}; p_1, p_2, \dots, p_{3N}) d^{3N} q d^{3N} p. \quad (11)$$

It is evident that for the typical statistical systems of $N \sim N_A \sim 10^{23}$ particles, calculation of such integrals is possible only if both functions w and f have a high degree of symmetry. (Even having all the particles identical does not always help.) This is why statistical physics is especially rich with approximate methods, and many simple-looking problems still evade exact solutions.

Finally, note that in the case of N particles, some degrees of freedom may not be random. For example, if a system is Hamiltonian (e.g., all inter-particle interactions are due to potential fields) and external conditions (e.g., volume) are constant, the total energy E of the system is exactly conserved. Moreover, if there are no external forces (say, we are discussing the set of all particles of an isolated star), the system total momentum \vec{P} and angular momentum \vec{L} are also conserved, and are reliably determined by initial conditions. However, in a typical situation the number of such degrees of freedom is limited, and at $N \gg 1$ their deterministic character does not affect noticeably the statistical approach results.

2.2. Density Matrix

Since quantum systems cannot be completely described by a set of classical variables, the definition of probability in them requires a special discussion. Quantum mechanics says that in arbitrary state of a statistical ensemble of similar quantum systems, the average (expectation) value of a function of the system state is defined by a formula more general than Eq. (7):

$$\langle F \rangle = \sum_{j,k} w_{j,k} F_{k,j}. \quad (12)$$

Here $F_{k,j}$ are the matrix elements of the quantum operator \hat{F} corresponding to the function F ,

$$F_{k,j} = \langle j | \hat{F} | k \rangle, \quad (13)$$

the double summation is over the same (but arbitrary) full set of basis functions $|j\rangle$, and coefficients $w_{j,k}$ form the so-called *density matrix*.³

Though Eq. (12) may be considered the density matrix definition, it is useful to have a look at a particular case when all systems of the quantum ensemble are in the same state α which may be presented as a linear superposition of the basis functions:

$$|\alpha\rangle = \sum_j c_j |j\rangle. \quad (14)$$

In such “*pure ensemble*”, the ensemble average of function F equals to its quantum-mechanical average in state α :

$$\langle F \rangle = \langle \hat{F} \rangle_\alpha = \langle \alpha | \hat{F} | \alpha \rangle = \sum_{j,k} c_j^* \langle j | \hat{F} | k \rangle c_k = \sum_{j,k} c_j^* c_k F_{j,k}. \quad (15)$$

Comparing this expression with Eq. (12), we see that for the pure ensemble the density matrix has a very simple form

$$w_{k,j} = c_j^* c_k, \quad (16)$$

with off-diagonal components ($n \neq m$) as large as the diagonal components. For example, in the simplest two-level system, the density matrix is

$$w = \begin{pmatrix} c_1^* c_1 & c_2^* c_1 \\ c_1^* c_2 & c_2^* c_2 \end{pmatrix} = \begin{pmatrix} |c_1|^2 & c_2^* c_1 \\ c_1^* c_2 & |c_2|^2 \end{pmatrix}, \quad (17)$$

and we see that the product its off-diagonal components, $(c_1^* c_2)(c_2^* c_1) = |c_1|^2 |c_2|^2$ is as large as that of the diagonal components.

However, the quantum coherence described by this fact is very vulnerable to perturbations. Indeed, let us have a look at the important case when the basis $|j\rangle$ is the set of energy eigenfunctions $|n\rangle$. In this case, the expansion coefficients c_n oscillate in time as

$$c_n = |c_n| \exp(-i \frac{E_n}{\hbar} t - i \varphi_n), \quad (18)$$

where E_n is the corresponding eigenenergy, and φ_j is an arbitrary constant. This means that while the diagonal terms of the density matrix are constant in time, its off-diagonal components are rapidly oscillating functions of time:

$$w_{n,n'} = c_n^* c_{n'} = |c_n| |c_{n'}| \exp\left\{-i \frac{E_{n'} - E_n}{\hbar} t\right\} \exp\{-i(\varphi_{n'} - \varphi_n)\}. \quad (19)$$

³ According to the matrix algebra, Eq. (12) may be also presented in the basis-independent form $\langle F \rangle = \sum_j (\hat{w} \hat{F})_{jj} = \text{Tr}(\hat{w} \hat{F})$, where w is called the *statistical operator*. Thus the density matrix $w_{k,j}$ is just the matrix of the statistical operator in the specific basis $|j\rangle$: $w_{k,j} = \langle k | \hat{w} | j \rangle$.

A minor perturbation (of either the initial condition or the system dynamics) may cause a significant shift of the phase difference, leading to a substantially different value of the second exponent in Eq. (20).

This is why in most cases, statistical ensembles of quantum particles are far from being pure (coherent). Moreover, in most cases a better approximation is given by the opposite limit of the completely *mixed ensemble* where all the phase differences ($\varphi_{n'} - \varphi_n$) are completely random (for $n \neq n'$), so that the off-diagonal matrix elements vanish. In this case each diagonal element $w_{n,n}$ of the density matrix have a simple physical sense of the probability to find the system in an eigenstate with energy E_n .

2.3. The Microcanonical Ensemble and the Basic Statistical Hypothesis

Let us start with the discussion of the simplest, “*microcanonical*” statistical ensemble which is a set of similar systems with virtually the same total energy E . (If we want a system of such set to belong to it indefinitely, it should be closed – see Sec. 1.2.) From the point of view of classical mechanics, we could fix E of a closed system exactly, but since in quantum mechanics energy of such system is quantized, it is more convenient to include into the ensemble all systems with eigenenergies E_n within a narrow interval $\Delta E \ll E$.

For this ensemble, the foundation of physical statistics, called *the basic statistical hypothesis* (as we will see below, replaces the entropy maximum postulate of thermodynamics) may be formulated as follows: in the thermodynamic equilibrium, all possible states within the range ΔE have equal probability. To make this statement quantitative, if the range includes M such states, then the probability of each of them

$$w_n = \frac{1}{M} = \text{const}, \quad (20)$$

the equation sometimes called the *microcanonical distribution*. Though in many theoretical constructs of statistical mechanics this distribution is derived from other axioms which look more plausible for their authors, I believe that Eq. (20) may be taken as the starting point of the statistical physics, supported “just” by the compliance of all its corollaries with experimental observations.

Nevertheless, it is always useful to give some thought to such fundamental principles. My own interpretation of the basic statistical hypothesis is that the (internal) energy E of a statistical system is its only substantial attribute which determines, in particular, the state’s probability at equilibrium.

2.4. Entropy and Information

Now let us find a suitable definition of entropy S of a microcanonical ensemble (for now, in equilibrium only). Since S is a measure of disorder, it should be related to the amount of information *lost* when the system goes from most definite state, say that with a definite wavefunction $|n\rangle$, into the equilibrium state described by Eq. (20), or vice versa, the amount of

information *necessary* to learn the exact state of your system, starting from its microcanonical distribution.

In the information theory, the amount of information necessary to make a choice between two states with equal *ab initio* probability is defined as

$$I(2) = \log_2 2 = 1. \quad (21)$$

This unit of information is called a *bit*. Now, if we need to make a choice between 4 such opportunities, it can be made in two similar steps (Fig. 1), each requiring one bit of information, so that the total amount of information necessary for the choice is

$$I(4) = 2I(2) = 2 = \log_2 4. \quad (22)$$

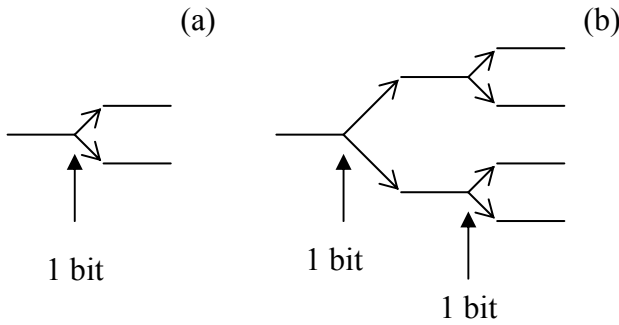


Fig. 2.1. The logarithmic trees of binary decisions for making a choice between (a) two and (b) four opportunities with equal probabilities.

An obvious extension of this process to the choice between $M = 2^m$ states gives

$$I(M) = mI(2) = m = \log_2 M. \quad (23)$$

This measure, if extended to any integer M ,⁴ is quite suitable for the definition of entropy at equilibrium, with the only difference that, following physics tradition, the binary logarithm is replaced with the natural one. This is of course just the change of units:⁵

$$S(M) \equiv \ln M = \frac{\log_2 M}{\log_2 e} = \ln 2 \times \log_2 M = \ln 2 \times I(M) \approx 0.693 I(M). \quad (24)$$

Using Eq. (20), we arrive at the canonical form of this relation (again, valid at the thermal equilibrium only!):

$$S = \ln \frac{1}{w_n} = -\ln w_n. \quad (25)$$

It is immediately evident that this definition satisfies the requirement of the entropy being an extensive thermodynamic function. Indeed, for two independent systems the joint probability is just a product of their partial probabilities, and hence, according to Eq. (25), their entropies just add up.

⁴ Such extension, leading to the fractional number of bits, is used in the statistical theory of information as well.

⁵ Note that in a Kelvin-degree-based system of units, e.g., SI (see Footnote 6 in Ch. 1), one bit of information corresponds to $\Delta S = k_B \ln 2 \approx 0.693 k_B$.

Now, let us discuss two evident points of discomfort with this definition of entropy. First, it depends on the accepted energy interval ΔE of the microcanonical ensemble, for whose width and exact position no exact guidance is offered. However, let us note that if the interval ΔE contains many levels, $M \gg 1$, then M , with a very small error (vanishing in the limit $M \rightarrow \infty$), may be replaced by the average number of energy levels in any such interval in the vicinity of E , and presented as

$$M = \Gamma(E)\Delta E, \quad (26)$$

where $\Gamma(E)$ is the density of states of the system:

$$\Gamma(E) \equiv \frac{d\Sigma(E)}{dE}, \quad (27)$$

$\Sigma(E)$ being the total number of eigenstates with energies below E . Plugging Eq. (26) into Eq. (24), we get

$$S = \ln M = \ln \Gamma(E) + \ln \Delta E, \quad (28)$$

so that the only effect of a particular choice of ΔE is a shift of entropy by a constant, and thermodynamics (see Ch. 1) shows that such a shift is insignificant for all measurable quantities.

Of course, this argument makes sense only for the cases when density of states $\Gamma(E)$ is so large that the range available for the appropriate choice of ΔE ,

$$\frac{1}{\Gamma(E)} \ll \Delta E \ll E, \quad (29)$$

is sufficiently broad. In order to get some feeling of the functions $\Gamma(E)$ and $S(E)$, let us consider a very simple but representative system: a set of N independent, similar harmonic oscillators with eigenfrequency ω . Quantum mechanics teaches us that the eigenenergy of such oscillator may take only discrete values,

$$\varepsilon = \hbar\omega(k + \frac{1}{2}), \quad k = 0, 1, 2, \dots \quad (30)$$

If ω is kept constant,⁶ the zero-point energy $\hbar\omega/2$ does not contribute to any thermodynamic properties of the system and can be ignored, so that we may take $\varepsilon = k\hbar\omega$. Let us carry out an approximate analysis of the system for the case when its average energy per oscillator,

$$\langle \varepsilon \rangle = \frac{E}{N}, \quad (31)$$

is much larger than the energy quantum $\hbar\omega$. For one oscillator, the number of states with energy ε below energy $E \gg \hbar\omega$ is evidently $\Sigma_1(E) \approx E/\hbar\omega$ (Fig. 2a). For two oscillators, all the possible values of the total energy $\varepsilon_1 + \varepsilon_2$ below E correspond to the points of a square grid within the triangle shown in Fig. 2b, giving $\Sigma_2(E) \approx (1/2) (E/\hbar\omega)^2$. For three oscillators, the possible values of the total energy $\varepsilon_1 + \varepsilon_2 + \varepsilon_3$ correspond to the points of the cubic mesh fitting inside the

⁶ Let me hope that you know about the famous Casimir effect arising due to the change of the zero-point energy with the frequency of EM radiation oscillators. We will see in Ch. 6 that the zero-point energy is also experimentally observable via the so-called “quantum fluctuations”.

pyramid shown in Fig. 2c, giving $\Sigma_3(E) \approx (1/6) (E/\hbar\omega)^3$, etc. It is clear now that for an arbitrary N the number of states is

$$\Sigma_N(E) \approx c_N \left(\frac{E}{\hbar\omega} \right)^N, \quad (32)$$

where coefficient $c_N = 1/N!$ has the sense of the hyper-volume of an N -dimensional right pyramid with unit sides.

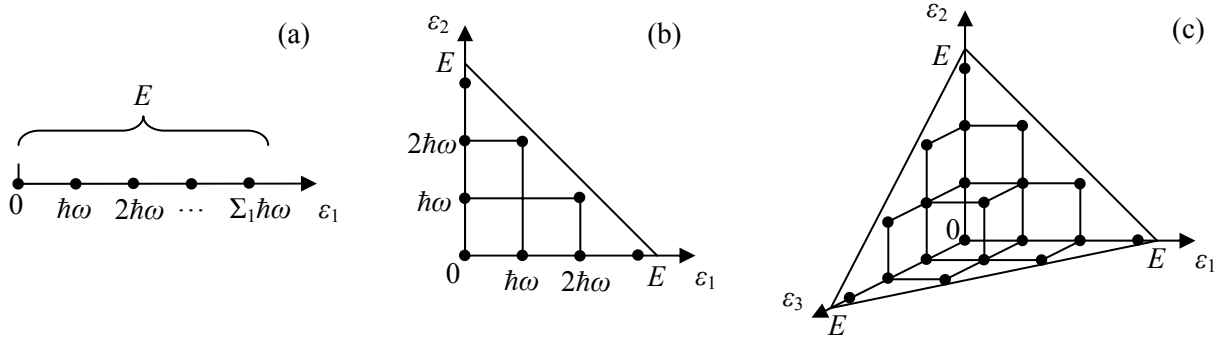


Fig. 2.2. Calculating functions $\Sigma_N(E)$ for the systems of (a) one, (b) two and (c) three quantum oscillators.

Differentiating Eq. (32), we get (in the limit $E/N\hbar\omega \rightarrow \infty$):

$$\Gamma(E) = \frac{d\Sigma_N(E)}{dE} = \frac{1}{(N-1)!} \frac{E^{N-1}}{(\hbar\omega)^N}, \quad (33)$$

so that

$$S(E) = \ln \Gamma(E) + \text{const} = (N-1) \ln E - N \ln(\hbar\omega) - \ln[(N-1)!] + \text{const}. \quad (34)$$

In the most interesting case of a statistical ensemble of many oscillators ($N \gg 1$), we can use the famous *Stirling formula* (in its crudest form, suitable for most purposes of statistical physics),

$$\ln(N!) \Big|_{N \rightarrow \infty} \rightarrow N(\ln N - 1) = N \ln \frac{N}{e}, \quad (35)$$

to simplify Eq. (34):

$$S(E) - \text{const} \approx N \ln E - N \ln(\hbar\omega) - N \ln \frac{N}{e} + \text{const} = N \ln \frac{eE}{N\hbar\omega} = N \ln \frac{e\langle \varepsilon \rangle}{\hbar\omega}. \quad (36)$$

We see that in our case ($\langle \varepsilon \rangle \gg \hbar\omega$, i.e. the logarithm in Eq. (36) is substantially larger than one), the density of states, in the limit $N \rightarrow \infty$, is exponentially large:

$$\Gamma(E) = e^S \sim \left(\frac{e\langle \varepsilon \rangle}{\hbar\omega} \right)^N, \quad (37)$$

so that both conditions (29) may be indeed satisfied within a very broad range of ΔE .

Actually, in our example we are just one step from a very interesting result. Indeed, according to thermodynamics (see Ch. 1), if the system volume and number of particles do not change, the derivative dS/dE is nothing more than the reciprocal temperature. Differentiating Eq. (36), we get

$$\frac{1}{T} = \frac{dS}{dE} = \frac{N}{E} = \frac{1}{\langle \varepsilon \rangle}. \quad (38)$$

Reading this result backwards, we see that (at least for the microcanonical ensemble we are studying now), the average energy $\langle \varepsilon \rangle$ of a harmonic oscillator equals T . As we will show in the next chapter, this is the correct asymptotic form of the exact result (given by the Bose-Einstein distribution), in the considered limit $\langle \varepsilon \rangle \gg \hbar\omega$. It is sort of surprising that we have been able to obtain the correct coefficient (unity) in this relation with such a crude calculation. (Actually, we would get the same result if we ignored the coefficients c_N altogether!) This is a very impressive demonstration of the extraordinary power of statistical physics.

2.5. Maxwell's Demon and Energy Consumption at Calculation

Another possible (and very popular) concern is the direct correspondence between the entropy and information given by Eq. (24). Some scientists still believe that there is more in the heat physics than just bare information theory, though to the best of my knowledge nobody has yet been able to refute any results following from that equation. Moreover, as early in 1867, J. C. Maxwell gave a wonderful example of the direct relation of these two notions.

Consider a volume containing just one molecule of gas, separated to two equal volumes with a partition and a door which may be opened and closed when necessary, apparently at no energy cost (Fig. 3a). If the door is open and the system is in thermodynamic equilibrium, we do not know which side of the door partition the molecule is. In the ensemble of similar systems like that, the disorder (and hence entropy) are maximal, and there is no way to get from it, on the average, useful mechanical energy.

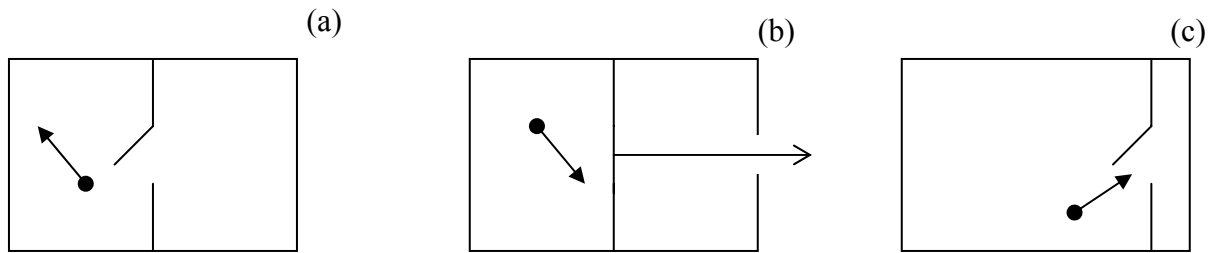


Fig. 2.3. The Maxwell's Demon paradox: the volume with a single molecule (a) before and (b) after closing the door, and (c) after opening the door in the end of the expansion stage.

Now, let us consider that we (or, in Maxwell's formulation, an omniscient Demon) know which side of the partition the molecule is currently located. Then we can close the door, so that molecule's impacts on the partition create, on the average, a pressure force directed toward the empty part of the volume (to the right in Fig. 3). Now we can get from the molecule a

mechanical work, say by allowing the pressure to move the partition to the right (Fig. 3b). After the partition is moved to the right end of the volume, we can open the door again (Fig. 3c), equalizing the pressure from both parts, and move the partition back to the middle without doing any substantial work. Then we can repeat the cycle again and again, and hence make the system to do unlimited useful work, fed only by information and thermal motion.

Let us calculate the maximum work per cycle made by this machine, assuming that it is constantly in thermal equilibrium with a heat bath of temperature T . The necessary knowledge of what exactly half of the volume contains molecule corresponds to exactly one bit, $I = 1$. According to Eq. (24) this means that by getting this information we are reducing entropy by $\Delta S_I = -\ln 2$. Now, it would be a mistake to plug this (negative) entropy change into Eq. (1.15). First, that equation is only valid for slow, reversible processes. Moreover (and more importantly), this equation, as well as its irreversible version (1.39) takes into account only the entropy change due to the heat flow $\Delta Q \leq T\Delta S$. The change ΔS_I does not belong to this category, and may be formally described by the change of the statistical ensemble – from one consisting of all similar systems (experiments) with the unknown location of the molecule, to the new ensemble consisting of the systems with the molecule in its certain (in Fig. 3, left) half. This procedure of redefining the statistical ensemble is the central point of the connection between the information theory and physics – in particular, at quantum measurements.

Now let us consider the slow expansion of the “gas” after the door had been closed. Now we can indeed use the reversible relation (1.17), and at the assumed isothermal conditions ($T = \text{const}$) we can readily integrate it over the whole expansion process, getting $\Delta Q = T\Delta S$. In the ultimate finite position, entropy should be the same as initially, before the door had been opened. (We again do not know where the molecule is.) This means that the entropy replenished, during the expansion, from the heat bath, is $\Delta S = -\Delta S_I = +\ln 2$, so that $\Delta Q = T\Delta S = T\ln 2$. Since by the end of the whole cycle the internal energy E of the system is the same as before, all this heat should go into the mechanical energy obtained during the expansion. Thus the obtained work per cycle (i.e. for each obtained information bit) is $T\ln 2$, or $k_B T_K \ln 2$ in practical units (about 4×10^{-21} Joule at room temperature).⁷

The smallness of that amount has left the Maxwell’s Demon paradox an academic exercise for more than a century. However, its discussion resumed in the 1970s in the context of energy consumption at calculations, and is still continuing. This revival is motivated by the fast (“Moore’s Law”) progress of digital integrated circuit technology, leading in particular, to a fast reduction of energy sent (dissipated, i.e. turned to heat) per one binary logic operation. In the currently dominating CMOS technology, this energy is close to

$$\Delta Q = CV_{DD}^2, \quad (39)$$

where V_{DD} is the power supply voltage (which determines the signal voltage swing), and C is the average capacitance of interconnects between logic gates, including contributions from wiring and transistor gates. The former contribution presently dominates, and can be crudely estimated as $C_0 L$ where L is the wire length and C_0 specific capacitance which is almost technology-independent and close to 2 pF/cm. For the current (“65-nm”) generation of CMOS technology,

⁷ Note that the work is vanishing at $T = 0$, so that, again, it may be obtained only if both necessary components, information *and* finite-temperature environment (heat bath) are in supply.

average L is of the order of 300 nm (i.e. $C \sim 6 \times 10^{-16}$ F), and $V_{DD} \sim 1$ V, so that $\Delta Q \sim 6 \times 10^{-16}$ J, i.e. exceeds $T \ln 2$ by about 5 orders of magnitude. Still, some engineers argue that the latter amount presents a fundamental limit and an insurmountable obstacle to the future progress of computing, so that the problem deserves a discussion.

In contrast to naïve thinking, computers do not *create* new information; they only reshape it, *loosing* some on the go. Indeed, digital computing may be always decomposed into logical operations, each of them performed by a certain logic gate. Some of them (e.g., logical NOT performed by inverters) do not change the amount of information. On the other hand, such logic gates as two-input AND or OR (or NAND or NOR or XOR) actually erase one bit at each operation, because they turn two input bits into one output bit (Fig. 4a). Exactly reversing the Maxwell's Demon argument, we arrive at the conclusion that such an *irreversible* logic operation should turn at least $T \ln 2$ of energy (provided by power supply) into heat. The detailed analysis of such loss has been carried out by R. Landauer.

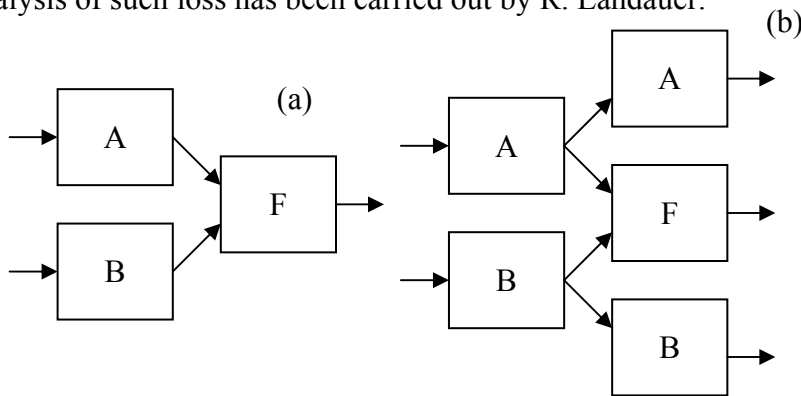


Fig. 2.4. Examples of (a) irreversible and (b) potentially reversible logic circuits. Each rectangle presents a circuit storing one bit of information.

However, very soon after that C. Bennett showed that it is possible to circumvent that energy loss by using only *reversible* logic operations.⁸ For that, one has to avoid erasure of any intermediate results, for example in the way shown in Fig. 4b. (In the end of the simulations the results can be “rolled back” to disappear, again without erasing a single bit.) Analyses have shown that the energy dissipation at such reversible calculation is not fixed by the performed function, but tends to zero as the calculation speed is decreased, so that the energy loss per bit may be less than the perceived “thermodynamic limit” $T \ln 2$.⁹ The price to pay for this ultralow dissipation is the enormous complexity of hardware necessary for storage and processing of all intermediate results. However, using irreversible gates sparingly, it may be possible in future to use the mostly reversible computing in future practical microelectronics.¹⁰

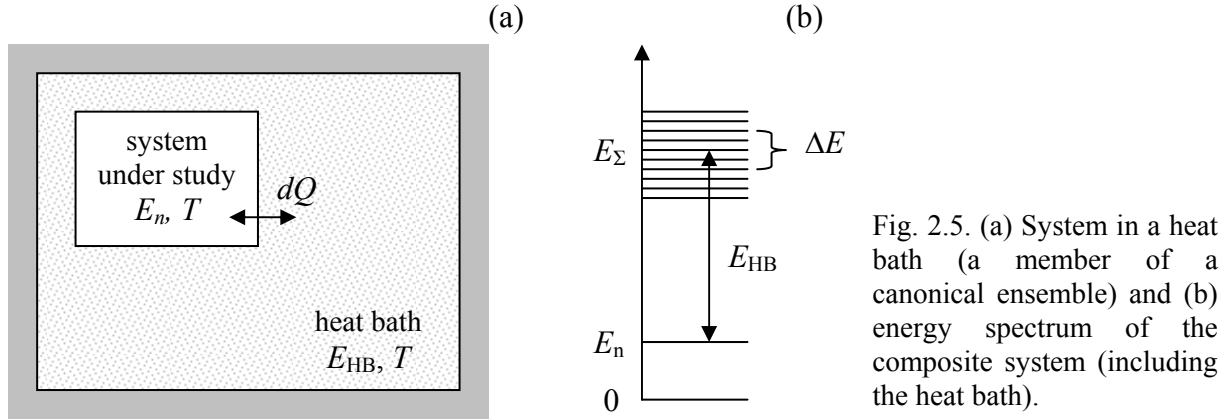
2.6. Canonical Ensemble and the Gibbs Distribution

(to be detailed)

⁸ A necessary condition for such operation is to have no power consumption at rest (with no logic operations running). While this is impossible in CMOS technology, more exotic electron devices (e.g., based on the Josephson effect or single-electron tunneling) offer such opportunity.

⁹ Another perceived “fundamental limit” $\Delta Q \times \Delta t > \hbar$, where Δt is the calculation time, has also turned to be wrong.

¹⁰ The situation is rather different for quantum computing which may be considered as a specific type of reversible computation. I will discuss this topic in the QM part of the notes.



$$E_{\Sigma} = E_n + E_{\text{HB}} = \text{const.}$$

$$\frac{1}{\Gamma(E)} \ll \Delta E \ll E \ll E_{\text{HB}}.$$

$$w_n = \text{const} \times \Gamma_{\text{HB}}(E_{\text{HB}})|_{E=E_n} \Delta E = \text{const} \times \Gamma_{\text{HB}}(E_{\Sigma} - E_n) \Delta E.$$

$$\ln w_n = \ln \Gamma_{\text{HB}}(E_{\Sigma} - E) + \text{const} = S_{\text{HB}}(E_{\Sigma} - E) + \text{const} \approx S(E_{\Sigma}) - \frac{dS_{\text{HB}}}{dE_{\text{HB}}}|_{E_n=0} E_n + \text{const}.$$

Using Eqs. (1.4), (1.5):

$$\ln w_n = -\frac{E_n}{T} + \text{const}.$$

$$w_n = C \exp\left\{-\frac{E_n}{T}\right\}.$$

(the Gibbs distribution). Normalization:

$$Z \equiv \frac{1}{C} = \sum_n \exp\left\{-\frac{E_n}{T}\right\}.$$

Entropy for an arbitrary distribution:

$$P = \frac{N!}{N_1! N_2! \dots N_M!}.$$

$$\begin{aligned} S &= \frac{\ln P}{N} = \frac{1}{N} \left[\ln(N!) - \sum_{n=1}^M \ln(N_n!) \right] \approx \frac{1}{N} \left[N \ln \frac{N}{e} - \sum_{n=1}^M N_n \ln \frac{N_n}{e} \right] \\ &= \ln N - \frac{1}{N} \sum_{n=1}^M N_n \ln N_n = - \sum_{n=1}^M \frac{N_n}{N} \ln \frac{N_n}{N}. \end{aligned}$$

$$S \rightarrow -\sum_{n=1}^M w_n \ln w_n = \sum_{n=1}^M w_n \ln \frac{1}{w_n}.$$

(reaches maximum in the case (25)).

Returning to the Gibbs distribution:

$$S = -\sum_n w_n \ln w_n = -\sum_n \frac{\exp\{-E_n/T\}}{Z} \left(-\frac{E_n}{T} - \ln Z \right) = \frac{E}{T} + \ln Z.$$

$$F \equiv E - TS = -T \ln Z.$$

$$\exp\left\{-\frac{F}{T}\right\} = Z = \sum_n \exp\left\{-\frac{E_n}{T}\right\}.$$

$$w_n = \frac{1}{Z} \exp\left\{-\frac{E_n}{T}\right\} = \exp\left\{\frac{F - E_n}{T}\right\}.$$

2.7. Grand Canonical Ensemble and Distribution

(to be detailed)

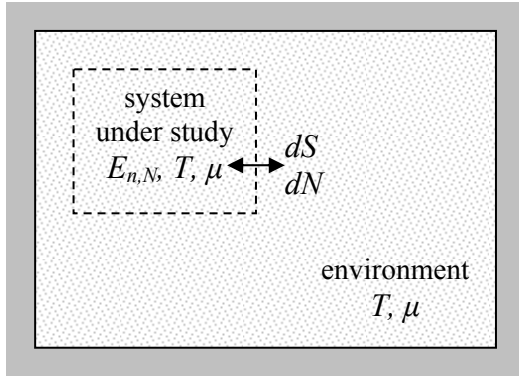


Fig. 2.6. A member of a grand canonical ensemble.

$$\ln w_{n,N} = \ln \Gamma_E(E_\Sigma - E_{n,N}, N_\Sigma - N) + \text{const} = S_E(E_\Sigma - E_{n,N}, N_\Sigma - N) + \text{const}$$

$$\approx S_E(E_\Sigma, N_\Sigma) - \frac{\partial S_E}{\partial T_E} \bigg|_{\substack{E_{n,N}=0 \\ N=0}} E_{n,N} - \frac{\partial S_E}{\partial N_E} \bigg|_{\substack{E_{n,N}=0 \\ N=0}} N + \text{const}.$$

From Eq. (1.50):

$$dS = \frac{1}{T} dE + \frac{p}{T} dV - \frac{\mu}{T} dN.$$

$$\ln w_{n,N} = S_E(E_\Sigma, N_\Sigma) - \frac{1}{T} E_{n,N} + \frac{\mu}{T} N + \text{const}.$$

$$w_{n,N} = C \exp \left\{ -\frac{E_{n,N}}{T} + \frac{\mu}{T} N \right\}.$$

(the grand canonical distribution). Normalization:

$$C = \frac{1}{\sum_{n,N} \exp \{ -E_{n,N} / T + \mu N / T \}} = \frac{1}{\sum_n \exp \{ -E_{n,N} / T \} \sum_N \exp \{ \mu N / T \}}.$$

$$S = -\sum_{n,N} w_{n,N} \ln w_{n,N} = -\ln C - \frac{\mu \langle N \rangle}{T} + \frac{E}{T}.$$

$$\Omega = E - TS - \mu \langle N \rangle = T \ln C.$$

$$w_{n,N} = \exp \left\{ \frac{1}{T} (\Omega + \mu N - E_{n,N}) \right\}.$$