

4.4.2 Simplifications for large N

To describe equilibrium properties of macroscopic bodies, statistical mechanics has to deal with the very large number N , of microscopic degrees of freedom. Actually, taking the *thermodynamic limit* of $N \rightarrow \infty$ leads to a number of simplifications, some of which are described in this section.

There are typically three types of N dependence encountered in the thermodynamic limit:

- *Intensive* quantities, such as temperature T , and generalized forces, e.g. pressure P , and magnetic field \vec{B} , are independent of N , i.e. $\mathcal{O}(N^0)$.
- *Extensive* quantities, such as energy E , entropy S , and generalized displacements, e.g. volume V , and magnetization \vec{M} , are proportional to N , i.e. $\mathcal{O}(N^1)$.
- *Exponential* dependence, i.e. $\mathcal{O}(\exp(N\phi))$, is encountered in enumerating discrete micro-states, or computing available volumes in phase space.
- Other asymptotic dependencies are certainly not ruled out a priori. For example, the Coulomb energy of N ions at fixed density scales as $Q^2/R \sim N^{5/3}$. Such dependencies are rarely encountered in every day physics. The Coulomb interaction of ions is quickly screened by counter-ions, resulting in an extensive overall energy. (This is not the case in astrophysical problems since the gravitational energy is not screened. For example the entropy of a black hole is proportional to the square of its mass.)

In statistical physics we frequently encounter sums or integrals of exponential variables. Performing such sums in the thermodynamic limit is considerably simplified due to the following results.

Summation of exponentials:

Consider the sum

$$\mathcal{S} = \sum_{i=1}^{\mathcal{N}} \mathcal{E}_i \quad , \quad (4.4.6)$$

where each term is positive, with an exponential dependence on N , i.e.

$$0 \leq \mathcal{E}_i \sim \mathcal{O}(\exp(N\phi_i)) \quad , \quad (4.4.7)$$

and the number of terms \mathcal{N} , is proportional to some power of N .

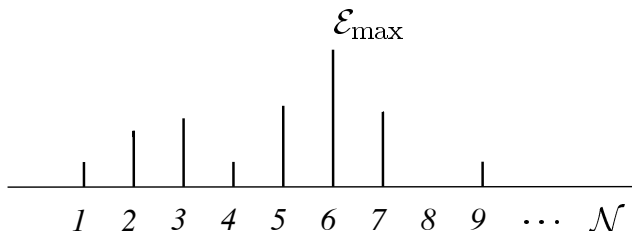


Figure 4.6: A sum over \mathcal{N} exponentially large quantities is dominated by the largest term.

Such a sum can be approximated by its largest term \mathcal{E}_{\max} , in the following sense. Since for each term in the sum, $0 \leq \mathcal{E}_i \leq \mathcal{E}_{\max}$,

$$\mathcal{E}_{\max} \leq \mathcal{S} \leq \mathcal{N}\mathcal{E}_{\max} . \quad (4.4.8)$$

An intensive quantity can be constructed from $\ln \mathcal{S}/N$, which is bounded by

$$\frac{\ln \mathcal{E}_{\max}}{N} \leq \frac{\ln \mathcal{S}}{N} \leq \frac{\ln \mathcal{E}_{\max}}{N} + \frac{\ln \mathcal{N}}{N} . \quad (4.4.9)$$

For $\mathcal{N} \propto N^p$, the ratio $\ln \mathcal{N}/N$ vanishes in the large N limit, and

$$\lim_{N \rightarrow \infty} \frac{\ln \mathcal{S}}{N} = \frac{\ln \mathcal{E}_{\max}}{N} = \phi_{\max} . \quad (4.4.10)$$

Saddle point integration:

Similarly, an integral of the form

$$\mathcal{I} = \int dx \exp(N\phi(x)) , \quad (4.4.11)$$

can be approximated by the maximum value of the integrand, obtained at a point x_{\max} which maximizes the exponent $\phi(x)$. Expanding the exponent around this point gives

$$\mathcal{I} = \int dx \exp \left\{ N \left[\phi(x_{\max}) - \frac{1}{2} |\phi''(x_{\max})| (x - x_{\max})^2 + \dots \right] \right\} . \quad (4.4.12)$$

Note that at the maximum, the first derivative $\phi'(x_{\max})$, is zero, while the second derivative $\phi''(x_{\max})$, is negative. Terminating the series at the quadratic order results in

$$\mathcal{I} \approx e^{N\phi(x_{\max})} \int dx \exp \left[-\frac{N}{2} |\phi''(x_{\max})| (x - x_{\max})^2 \right] \approx \sqrt{\frac{2\pi}{N|\phi''(x_{\max})|}} e^{N\phi(x_{\max})} , \quad (4.4.13)$$

where the range of integration has been extended to $[-\infty, \infty]$. The latter is justified since the integrand is negligibly small outside the neighborhood of x_{\max} .

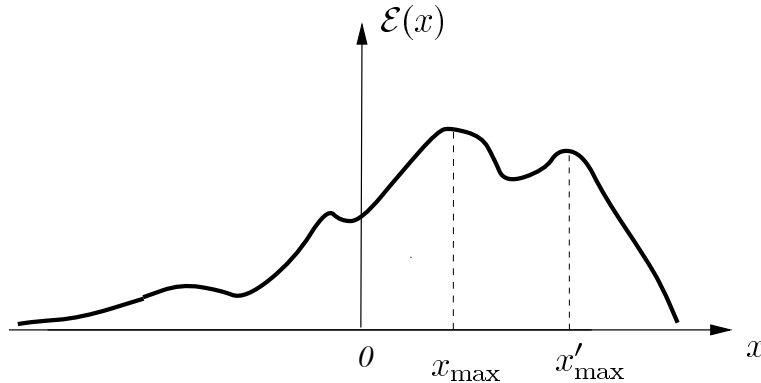


Figure 4.7: Saddle point evaluation of an ‘exponential’ integral.

There are two types of corrections to the above result. Firstly, there are higher order terms in the expansion of $\phi(x)$ around x_{\max} . These corrections can be looked at perturbatively, and lead to a series in powers of $1/N$. Secondly, there may be additional local maxima for the function. A maximum at x'_{\max} , leads to a similar Gaussian integral that can be added to Eq. (??). Clearly such contributions are smaller by $\mathcal{O}(\exp\{-N[\phi(x_{\max}) - \phi(x'_{\max})]\})$. Since all these corrections vanish in the thermodynamic limit,

$$\lim_{N \rightarrow \infty} \frac{\ln \mathcal{I}}{N} = \lim_{N \rightarrow \infty} \left[\phi(x_{\max}) - \frac{1}{2N} \ln \left(\frac{N|\phi''(x_{\max})|}{2\pi} \right) + \mathcal{O}\left(\frac{1}{N^2}\right) \right] = \phi(x_{\max}) \quad . \quad (4.4.14)$$

The *saddle point* method for evaluating integrals is the extension of the above result to more general integrands, and integration paths in the complex plane. (The appropriate extremum in the complex plane is a saddle point.) The simplified version presented above is sufficient for our needs.