

Theoretische Physik IV: Statistische Mechanik, Exercise 9

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1. Stirling's formula (Oral)

Here you derive the famous and (at least in statistical physics) ubiquitous approximation

$$n! \sim \left(\frac{n}{e}\right)^n \sqrt{2\pi n} \quad \text{for } n \in \mathbb{N}, n \rightarrow \infty \quad (1)$$

which is commonly referred to as *Stirling's formula*. To do this, consider the representation

$$n! = \Gamma(n+1) = \int_0^\infty x^n e^{-x} dx = \int_0^\infty \exp(n \ln x - x) dx \quad (2)$$

in terms of the Γ -function. Expand the logarithm $n \ln x - x$ of the integrand around its sharp maximum for $n \gg 1$ and evaluate the resulting Gaussian integral.

2. Fermionic and bosonic distribution functions (Oral)

In this exercise we re-derive the H -theorem for particles that obey bosonic and fermionic statistics to end up with the corresponding distribution functions. In the lecture was shown that for *classical* particles the one-particle density f satisfies the Boltzmann equation

$$\partial_t f + \dot{\mathbf{q}} \cdot \nabla_{\mathbf{q}} f + \dot{\mathbf{p}} \cdot \nabla_{\mathbf{p}} f = \partial_t f|_S \quad (3)$$

where $\partial_t f|_S$ describes the change of f due to scattering of the particles. For particle-particle scattering the expression

$$\partial_t f|_S = - \int d^3 p' d^3 p_1 d^3 p'_1 w_{\mathbf{p}', \mathbf{p}'_1; \mathbf{p}, \mathbf{p}_1} X(\mathbf{p}, \mathbf{p}_1, \mathbf{p}', \mathbf{p}'_1) \quad (4)$$

was motivated, where $X(\mathbf{p}, \mathbf{p}_1, \mathbf{p}', \mathbf{p}'_1) = f(\mathbf{p})f(\mathbf{p}_1) - f(\mathbf{p}')f(\mathbf{p}'_1)$. Now we consider *indistinguishable quantum particles* — they are defined by their statistics, that is, their behaviour upon interchange of identical particles. In the ansatz of *molecular chaos* the statistics can be incorporated via

$$X^\pm(\mathbf{p}, \mathbf{p}_1, \mathbf{p}', \mathbf{p}'_1) = f^\pm(\mathbf{p})f^\pm(\mathbf{p}_1) [1 \pm f^\pm(\mathbf{p}')] [1 \pm f^\pm(\mathbf{p}'_1)] - f^\pm(\mathbf{p}')f^\pm(\mathbf{p}'_1) [1 \pm f^\pm(\mathbf{p})] [1 \pm f^\pm(\mathbf{p}_1)] \quad (5)$$

where X^+ (X^-) describes bosons (fermions). Thermodynamic equilibrium demands $\partial_t f_0^\pm|_S = 0$ where f_0^+ (f_0^-) is called *Bose-Einstein statistics* (*Fermi-Dirac statistics*).

- (a) Derive the H -theorem for both bosonic and fermionic statistics. To do this, consider the generalized H -functional

$$H^\pm[f](t) := \int d^3p [f \ln f \mp (1 \pm f) \ln(1 \pm f)] \quad \text{where } f = f(p, t). \quad (6)$$

That is, show that $\partial_t H^\pm|_S \leq 0$ by using the symmetries of $w_{\mathbf{p}', \mathbf{p}'_1; \mathbf{p}, \mathbf{p}_1}$ and the definition of $X^\pm(\mathbf{p}, \mathbf{p}_1, \mathbf{p}', \mathbf{p}'_1)$.

- (b) Argue that $\partial_t H^\pm[f_0^\pm]|_S = 0$ implies $\ln\left(\frac{f_0^\pm}{1 \pm f_0^\pm}\right) = \frac{\mu}{k_B T} - \frac{\varepsilon(\mathbf{p})}{k_B T}$ for $\mu \in \mathbb{R}$, vanishing total momentum $p_0 = 0$ and energy $\varepsilon(p) = p^2/2m$.

Hint: You are allowed to choose the occurring constants to match the required form above. You are *not* asked to show that μ and T can be interpreted as chemical potential and temperature, respectively.

- (c) Derive the Bose-Einstein and Fermi-Dirac statistics $f_0^\pm(p)$.

3. Simulation of one-dimensional gas (Written)

In this exercise we illustrate the emergence of *macroscopic* thermodynamic properties by simulating the *microscopic* dynamics of a many-body system. To master this task, you may use the high level programming language or CAS of your choice. The sample solution as well as the technical hints below refer to **Mathematica**. Please note that there are **Mathematica** installations available on the physics CIP-pool computers.

Consider a one-dimensional system with N particles at positions $q_i \in \mathbb{R}$ and (conjugate) momenta $p_i \in \mathbb{R}$, $i = 1, \dots, N$. Two particles interact via the (smooth) van der Waals potential V_{vdW} . The gas is trapped in the global potential V_{T} . Then the Hamiltonian reads

$$\mathcal{H} = \sum_i \frac{p_i^2}{2m} + \sum_i V_{\text{T}}(q_i) + \sum_{i>j} V_{\text{vdW}}(q_i, q_j) \quad (7)$$

where $\sum_{i>j}$ denotes the sum over all pairs (i, j) and m is the particles' mass. The van der Waals potential is defined as

$$V_{\text{vdW}}(q_i, q_j) := \frac{\lambda}{1 + \rho(q_i - q_j)^6} \quad (8)$$

with the fixed parameters $\lambda, \rho \in \mathbb{R}_0^+$. The trapping potential can be chosen *harmonic* ($n = 2$) or *anharmonic* ($n = 4$):

$$V_{\text{T}}(q_i) := \gamma (q_i)^n, \quad n = 2, 4 \quad (9)$$

with $\gamma \in \mathbb{R}_0^+$.

- (a) Derive the equations of motion for both trapping potentials ($n = 2, 4$). What does $|V_{\text{vdW}}(q_i, q_j)| < \infty$ for all $q_i, q_j \in \mathbb{R}$ tell you about the behaviour of the particles?

- (b) Derive the time evolution of the center of mass $Q := \frac{1}{N} \sum_i q_i$ for the harmonic ($n = 2$) trap analytically. Can you do the same for the anharmonic ($n = 4$) trap?
- (c) For the sake of simplicity set $m = 1$, $\gamma = 1/n$, $\lambda = 1/6$, and $\rho = 100$. Write a program that integrates the equations of motion for $0 \leq t \leq 100 = t_{\max}$ and N particles ($n = 2, 4$). As initial conditions choose uniformly distributed positions $q_i(t = 0) \in [q_{\min}, q_{\max}]$ and momenta $p_i(t = 0) \in [p_{\min}, p_{\max}]$.
- (i) Plot for $N = 100$, $[q_{\min} = 1.9, q_{\max} = 2.1]$ and $[p_{\min} = -0.01, p_{\max} = 0.01]$ the center of mass motion $Q(t)$. Do this for both, the harmonic and the anharmonic trap. Compare the result for $n = 2$ with the analytic one.
- (ii) Plot for the anharmonic trap, $N = 100$ and the same initial conditions as above the average kinetic energy $E_{kin}(t) := \frac{1}{N} \sum_i \frac{p_i^2(t)}{2m}$. How long does it take to equilibrate?
- (iii) Let t_e be the equilibration time. Approximate the mean of an observable $X(t)$ via

$$\bar{X} \approx \frac{1}{t_{\max} - t_e} \int_{t_e}^{t_{\max}} X(t) dt \quad (10)$$

and compute the standard deviation $\sigma_E := \sqrt{\text{Var}[E_{kin}]} = \sqrt{(E_{kin} - \bar{E}_{kin})^2}$. Do this for different particle numbers $N \leq 100$ and plot $\sqrt{N} \sigma_E(N) (\bar{E}_{kin})^{-1}$ as a function of N . In addition, measure the time required for the solution of the equations of motion for the different particle numbers N . What do you observe? How does your result for $\sqrt{N} \sigma_E(N) (\bar{E}_{kin})^{-1}$ motivate the macroscopic description of thermodynamics? Based on your time measurements for $N \leq 100$, give an estimate how long an analogous computation for *one mole* ($N = 6 \cdot 10^{23}$) of this gas would take.

Please hand in your derivations as well as the plots and your conclusions. If you encounter any technical problems feel free to ask your tutor. Here are some notes regarding **Mathematica**:

- Detailed information on all **Mathematica** functions can be found online: <http://reference.wolfram.com/mathematica/guide/Mathematica.html>
- In **Mathematica** the evaluation of an expression is initiated via **Shift+Enter**.
- You can define vectors of functions $q_i(t)$ or $p_i(t)$ with variable length **NN** via

```
qvec=Table[Subscript[q, i][t], {i, NN}];
pvec=Table[Subscript[p, i][t], {i, NN}];
```

- Random initial conditions can be defined via

```
inq=Table[Subscript[q, i][0]==Random[Real, InitRangeQ], {i, NN}];
inp=Table[Subscript[p, i][0]==Random[Real, InitRangeP], {i, NN}];
```

where $\text{InitRangeQ}=\{q_{\min}, q_{\max}\}$ and $\text{InitRangeP}=\{p_{\min}, p_{\max}\}$ define the initial ranges for q_i and p_i .

- You can define the differential equations via

```
sysq=Table[D[Subscript[q, i][t],t]==<EOM>,{i,NN}];  
sysp=Table[D[Subscript[p, i][t],t]==<EOM>,{i,NN}];
```

where **D** denotes the derivative with respect to **t** and for <EOM> the right-hand side of the equations of motion is to be substituted.

- You can solve the equations of motion numerically via

```
sol=NDSolve[Join[sysq,sysp,inq,inp],  
Join[qvec,pvec],{t,0,tmax},MaxSteps->10^6];
```

where the solutions are stored in **sol**.

- You can plot e.g. the center of mass position via

```
Plot[Sum[Subscript[q, i][t]/NN,{i,NN}]/.sol,{t,0,tmax}]
```

- You can measure the time for evaluating an expression <expression> via

```
AbsoluteTiming[<expression>]
```