Lectures notes on Advanced Computational Statistical Physics

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Introduction

In the 19th century, classical mechanics, rooted in Newton's laws, dominated physics. Pierre-Simon Laplace famously articulated the deterministic worldview: given the initial conditions of a system, its future could be perfectly predicted through precise mathematical equations. This perspective treated the universe like a clockwork machine, where every event followed from the initial state.

However, as the study of thermodynamics and many-particle systems advanced, the limits of this purely deterministic approach became clear. Statistical physics emerged to address these complexities, particularly through the work of James Clerk Maxwell and Ludwig Boltzmann. Their pioneering contributions, such as Maxwell's velocity distribution in gases and Boltzmann's statistical interpretation of entropy, introduced probabilistic methods to understand the behavior of large ensembles of particles.

In this new framework, the precise motion of individual particles became less important; instead, statistical averages and distributions described macroscopic properties like temperature and pressure. While Laplace envisioned a universe governed by strict determinism, statistical physics embraced the unpredictability inherent in large systems, marking a profound shift in understanding.

This shift continued to resonate into the 20th century, influencing the work of physicists like Philip W. Anderson. Anderson famously argued that "more is different," suggesting that the behavior of complex systems cannot be fully understood by analyzing individual components alone. This echoes the insights of 19th-century statistical physics, where collective behavior emerged from many interacting parts, challenging the reductionist views of classical mechanics.

In summary, while classical mechanics remained essential for describing deterministic systems, the development of statistical physics in the 19th century introduced a probabilistic approach that transformed our understanding of many-body systems and laid the groundwork for modern physics.

I. Computational Statistical Physics

Computational methods allow us to simulate these complex systems directly, providing detailed insights into their behavior. Using modern computing power, scientists can model the interactions of millions, or even billions, of particles, making it possible to observe emergent phenomena such as phase transitions, critical behavior, and chaotic dynamics. This computational approach helps us overcome the "many-body" problem, where the sheer number of interactions in a system defies exact solutions.

One reason computational statistical physics is so powerful is that it can handle systems that are analytically intractable. For instance, systems with strong correlations between particles or those far from equilibrium, which are difficult to study using traditional methods, can be simulated using Monte Carlo techniques, molecular dynamics, and other algorithms.

Additionally, computational approaches enable the study of phenomena at different scales—from the atomic scale, where quantum effects dominate, to macroscopic scales governed by classical statistical physics. This versatility allows for a deeper understanding of both microscopic mechanisms and their macroscopic consequences, bridging the gap between theoretical models and real-world systems.

In essence, computational statistical physics allows us to explore systems that are too complex for exact solutions, providing a practical and powerful way to study emergent behavior, phase transitions, and non-equilibrium systems. By leveraging the power of computers (which is increasing exponentially since the second half of the 19th century Fig. 1.1), it opens up new frontiers for understanding the vast complexity of the physical world, which neither classical mechanics nor early analytical statistical methods could fully address.

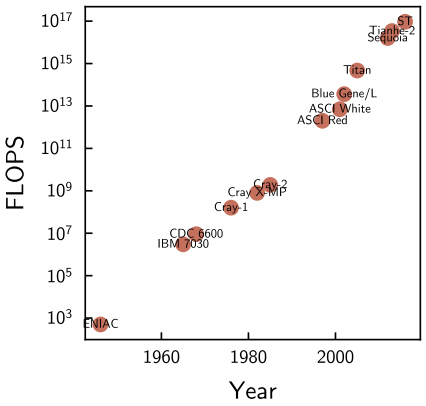

Figure 1.1 – Number of Floating points operations evolution for the biggest supercomputer

II. Invariant Measures and Ergodicity

In statistical physics, the concept of an invariant measure plays a crucial role in understanding the long-term behavior of dynamical systems, and the symetry of the system (Noether's theorem). One of the main goals of computational statistical physics is to find algorithms preserving the invariant measure of the systems we are studying. For example we will see that the Euler algorithm is not a good choice for simulating Hamiltonian systems, as it does not conserve the energy of the system, as opposed to the Verlet algorithm, which is based on clever considerations of the symplectic[1] structure of the phase space.

Ergodicity is another important concept in statistical physics, which ensures that the system explores the entire phase space in the long run. Which results in one of the most important hypothesis in computational statistical physics, the ergodic hypothesis, which states that the time average of a system is equal to its ensemble average (limit cases CITE).

[1] Refers to the Hamiltonian Formulation of classical mechanics

Molecular Dynamics

I. Hamiltonian Dynamics

A. Hamiltonian Formalism

The Legendre transformation of the Lagrangian allows us to define the Hamiltonian of a system, which is a function of the generalized coordinates q_i and the generalized momenta p_i of the system (see CITE). The Hamiltonian is defined as :

$$H \overset{\text{def}}{=} \frac{\mathbf{p}^T \mathbf{M}^{-1} \mathbf{p}}{2} + U(q)$$

with $U(q)$ the potential energy of the system and $\mathbf{M}$ the mass matrix of the system. The equations of motions can then be written using the Euler-Lagrange equations :

$$\begin{cases} \dot{q} = \frac{\partial H}{\partial p} \\ \dot{p} = -\frac{\partial H}{\partial q} \end{cases}$$

This can be written in a more compact matrix form :

$$\begin{pmatrix} \dot{\mathbf{q}} \\ \dot{\mathbf{p}} \end{pmatrix} = \mathbf{J} \nabla H(\mathbf{p}, \mathbf{q})$$

with

$$\mathbf{J} = \begin{pmatrix} 0 & \mathbf{I} \\ \mathbf{I} & 0 \end{pmatrix}$$

These type of non linear equations can only be locally, but since the systems are Hamiltonian we can unearth the global existence and uniqueness of the solutions. Indeed we just need to show that using the energy constraints of the system the solutions are bounded for all time. For the impulsion this is trivial considering a potential global minimum :

$$\frac{\mathbf{p}^T \mathbf{M}^{-1} \mathbf{p}}{2} \leq E_0 - U_{min}$$

for the position we just need an assumption on the level sets of the potential energy.

$$\Sigma_\alpha = \mathbf{q} | U(\mathbf{q} = \alpha)$$

If these lebel are bounded then the solutions are bounded for all time. This is not the case for all potentials, this is why for solving this kind of equations we will add sometimes confining potentials to the system.

B. Map Flow

Since the Hamiltonian equations are solvable, it seems natural to define a map flow $\mathcal{F}$ such that for an initial condition z_0 and a considered point z_t we have :

$$\mathbf{z}_t = \mathcal{F}_t(\mathbf{z}_0)$$

This flow map is obviously invertible and Hamiltonian conservative. The key of numerical integration is then to approximate the true flow map of the system by the numerical flow map $\mathcal{T}$ such that the physical properties of the system are conserved over time.

Considering the linear system for the differentiation :

$$\frac{\mathrm{d}\mathbf{z}}{\mathrm{d}t} = f(\mathbf{z}) = A\mathbf{z} \tag{2.1}$$

One way to solve this equation is to use the matrix exponential :

$$\mathbf{z}_t = \exp(At)\mathbf{z}_0$$

Then it appears that the flow map is given by :

$$\mathcal{F}_t(\mathbf{z}) = \exp(tA)\mathbf{z} \tag{2.2}$$

C. Sympletic Form

a) Volume Preservation

One of the most important properties of the flow map is the preservation of the volume in the phase space. Indeed,for a Hamiltonian system we have thanks to Liouville's theorem the volume of a given sets of solution governed by Eq. (2.1) is preserved over time if

$$\nabla \cdot f = 0 \,.$$

It is easy to show that for a Hamiltonian system :

$$\nabla \cdot f = \nabla \cdot \begin{pmatrix} 0 & \mathbf{I} \\ \mathbf{I} & 0 \end{pmatrix} \nabla H = 0$$

Due to the $\mathcal{C}^2$ property of the Hamiltonian. The main consequence of this property is that the flow map is volume preserving, which has to be a important property of the integration algorithm to approximate the flow map.

Volume preservation is a key prroperty since it ensures that the numerical integration keeps the hamiltonian structure of the system, following the loiouville theorem i.e the conservation of the phase space volume along particles trajectories in the phase space.

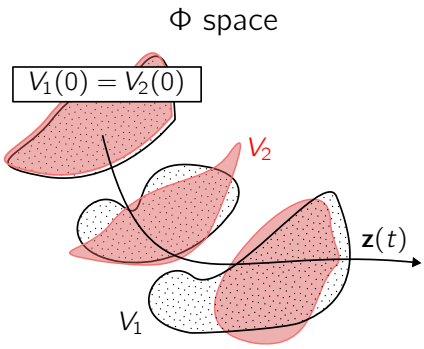

Figure 2.1 – Volume conservation for the true Hamiltonian in black and the approximated Hamiltonian in red

b) Sympletic Property

The sympletic property of the flow map is another important property of the Hamiltonian system. Indeed, the sympletic property of the flow map is defined as :

$$\mathcal{F}_t^T J \mathcal{F}_t = J$$

With $J = \begin{pmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 0 \end{pmatrix}$ the sympletic matrix. This property leeads to the conservation of the volume of the phase space, indeed we have for the jacobian associated with the map : $|\mathcal{F'}_t|^2 = 1$.

One intersting point of symplectic maps is that they form a group (they preserved the composition) which can be used to build other more complex symplectic maps. For example to increase the order of sympletic integrators $\mathcal{G}_h$ approximating the flow map $\mathcal{F}_h$, we can also split wut Hamiltonian just dependant of the impulsion or the position. This is called the splitting method, which is based on the Trotter expansion of the flow map (Find sympletic form of splitted hamiltonian).

D. Error Analysis for Hamiltonian splitting

a) Lie Derivatives and Poisson Brackets

Lie Derivatives

In the case of a non-Linear Hamiltonian system, the flow map can be approximated by the Lie derivative of the Hamiltonian, we would like to find again the conveninant results :

$$\mathcal{F}_t = \exp(tA)\mathbf{z}$$

Let's consider a functionnal Φ f the phase space, the Lie derivative of Φ is defined as :

$$\mathcal{L}_f \Phi = \nabla \Phi \cdot f$$

This is a generalization of the directional derivative to the phase space. Expanding the Φ map in a Taylor series we have :

$$\Phi(\mathbf{z}(t)) = \sum_i \frac{t^i}{i!}(\mathcal{L}_f^i\Phi)(\Phi(\mathbf{0})) = \exp(t\mathcal{L}_f)(\Phi(\mathbf{0}))$$

Applying this along the trajctory gives us the following map :

$$\mathcal{F}_t(\mathbf{z}) = \exp(t\mathcal{L}_f)(\mathbf{z})$$

As we wanted.

Poisson Brackets

A common notation introduced in Hamiltonian mechanics is the Poisson bracket, which is defined as :

$$\{g_1, g_2\} = \sum_{i=1}^{N}(\frac{\partial g_1}{\partial q_i}\frac{\partial g_2}{\partial p_i} - \frac{\partial g_2}{\partial q_i}\frac{\partial g_1}{\partial p_i}) = \nabla g_1^T \mathbf{J}\nabla g_2$$

Considering a smoooth scalar value function F of the phase space, we can show that the Lie derivative of F is given by the Poisson bracket of F and the Hamiltonian :

$$\mathcal{L}_{\mathbf{J}\nabla H}F = \mathcal{L}_H F = \{F, H\}$$

Poisson brackets can be related to the Lie derivating noticing that for every real valued function f:

$$[\mathcal{L}_{H_1}, \mathcal{L}_{H_2}]f = \mathcal{L}_{\{H_1,H_2\}}f$$

b) Error Analysis for non Commuting Hamiltonian

The main idea behinds this study is to consider integration method as a splitting of the Hamiltonian into several parts oftenly independant of one of the two system of coordinates $(\mathbf{q}, \mathbf{p})$, as we will see further. The poisson brackets are linear with respect to the Hamiltonian, which allows us to write the following considering $H = H_1 + H_2$,

$$\mathcal{L}_H = \mathcal{L}_{H_1} + \mathcal{L}_{H_2}$$

The flow map of the system is then defined as : $\mathcal{F}_t(\mathbf{z}) = e^{t()\mathcal{L}_{H_1}+\mathcal{L}_{H_2})}\mathbf{z}$

The splitting method has the following flow map :

$$\mathcal{G}_t h = e^{h\mathcal{L}_{H_1}}e^{h\mathcal{L}_{H_2}}$$

Which is not the same as the true flow map. To evaluate the error done considering the splitted Hamiltonian, we can use the Baker-Campbell-Hausdorff formula [CITE] and the correspondance between the Lie derivative and the Poisson bracket unearthing :

$$e^{h\mathcal{L}_{H_1}}e^{h\mathcal{L}_{H_2}} = e^{h\mathcal{L}_{\tilde{H}_h}}$$

With $\tilde{H}_h$ the *shadow Hamiltonian* :

$$\tilde{H}_h = H_1 + H_2 + \frac{h}{2}\{H_1, H_2\} + \frac{h^2}{12}(\{H_1\{H_1, H_2\}\} - \{H_2\{H_1, H_2\}\})\dots$$

From this we can easily understand that as long as the two splitted Hamiltonian do not commute, we have at least an linear error (on example is the sympletic Euler Method). One way to do that, is to find a split with commutating hamiltonian, or to split H into three hamiltonian such that that the linear term vanishes (such as the Velvet velovity & position method). The main indea behind this development was to show that the flow map $\mathcal{F}_t$ we approximate using the other $\mathcal{G}_t$ stands in the splitting method for an exact solution to a other (but similar) hamiltonian system.

To put in a nutshell the splitting method allows us to build sympletic integrator using Hamiltonian transformations. Not all intersteing integrators have sympletic structures, but they should all conserve volume in the phase space.

II. Time Integration

Here we will restrict our study to linear system. To perform time integration, we discretize time into small intervals δt . At each time step $t_{n+1} = n\delta t$, we approximate the change in the system using matrix iteration.

$$\begin{pmatrix} x(n\delta t) \\ y(n\delta t) \end{pmatrix} = \mathcal{T}^n(\delta t)\begin{pmatrix} x(0) \\ y(0) \end{pmatrix}$$

The goal is then to find the correct matrix such that iterating over time will not change the invariance of the system. To fit the previous notations the flow map can be defined as :

$$\mathcal{F}_{\delta t}(\mathbf{z}) = T(\delta t)\mathbf{z}$$

with $\mathcal{F}_{\delta t}$ a volume conservative flow map.

A. Application to the Harmonic Oscillator

$$\ddot{x} - \omega^2 x = 0$$

a) Exact Propagator

For the harmonic oscillator, the time evolution is well known which is useful to test the time integration algorithms. Indeed, we got :

$$\begin{pmatrix} x(\delta t) \\ \dot{x}(\delta t) \end{pmatrix} = \mathcal{T}(\delta t)\begin{pmatrix} x(0) \\ \dot{x}(0) \end{pmatrix}$$

With

$$\mathcal{T}(\delta t) = \begin{pmatrix} \cos(wt) & \frac{1}{w}\sin(wt) \\ w\sin(wt) & \cos(wt) \end{pmatrix}$$

In the next analysis we will use a dimensionless time $\tau = \omega t$, a dimensionless position $\xi = \sqrt{\frac{k}{k_B T}}x$ and a dimensionless impulsion $\Pi = \sqrt{\frac{1}{mk_bT}}p$, which leads to the following time Propagator :

$$\mathcal{F}_{\delta\tau} = \mathcal{T}(\delta\tau) = \begin{pmatrix} \cos(\delta\tau) & \sin(\delta\tau) \\ -\sin(\delta\tau) & \cos(\delta\tau) \end{pmatrix} = \exp(\mathbf{J}\tau)$$

Here we related as did previously the flow map to the derivative operation for our system. For the Hamiltonian we find :

$$H = \frac{\mathcal{H}}{k_B T} = \frac{1}{2}(\Pi^2 + \xi^2)$$

Then let's consider a microstate of the system $|\tau\rangle = \begin{pmatrix} \xi(\tau) \\ \Pi(\tau) \end{pmatrix}$ The time evolution of the system is given by the following equation :

$$|\tau + \delta\tau\rangle = \mathcal{T}(\delta\tau)|\tau\rangle$$

With the unitary propagation matrix

$$\mathcal{T}(\delta\tau) = \begin{pmatrix} \cos(\delta\tau) & \frac{1}{\omega}\sin(\delta\tau) \\ -\omega\sin(\delta\tau) & \cos(\delta\tau) \end{pmatrix}$$

Solving the characteristic equation $\|\mathcal{T} - \lambda I| = 0$, we unearth the eigenvalues.

$$\lambda_\pm = \exp(\pm i\delta\tau),$$

Considering the two **orthogonal** eigenvectors $|\pm\rangle$, we easily show that :

$$|n\delta t\rangle = \mathcal{T}(\delta t)^n|0\rangle = a_+\lambda_+^n|+\rangle + a_-\lambda_-^n|-\rangle$$

Considering the initial decomposition

$$|0\rangle = a_+|+\rangle + a_-|-\rangle$$

Then we can easily show that :

$$\begin{aligned}\frac{E}{k_b T} &= \frac{1}{2}\langle n\delta\tau | n\delta\tau\rangle \\ &= \frac{1}{2}\left(|a_+|^2|a-+|^2\right)\mathcal{T}(\delta t)^n \\ &= \frac{1}{2}\langle 0|0\rangle\end{aligned}$$

Which shows that the energy is conserved over time. We can also show an interesting result about the conserved quantities :

$$\begin{aligned}\langle 0|A|0\rangle &= \langle\tau|A|\tau\rangle \\ &\Rightarrow A \equiv \mathcal{T}^\dagger A \mathcal{T} \\ &\Rightarrow A \propto H\end{aligned}$$

b) Euler Algorithm & Propagator

The Euler algorithm is the simplest algorithm to perform time integration, based on the first order approximation in Taylor expansion. The expolicit non sympletic Euler algorithm is given by the following flow map :

$$\mathcal{G}^{\text{euler}}_{\delta\tau} = I - S\delta\tau$$

With S veryfing

$$\frac{\mathrm{d}\mathbf{z}}{\mathrm{d}\tau} = S\mathbf{z}$$

One can remark that for volume conservation the map should verify the following property :

$$\det(I - S\delta\tau) = 0$$

, which is generally not the case in physical system were the eigen values of S are oftenly pure imaginary. If we write the propagation matrix for the Euler algorithm, we obtain the following :

$$\mathcal{T}(\delta\tau) = \begin{pmatrix} 1 & \delta\tau \\ -\omega^2\delta\tau & 1 \end{pmatrix}$$

Which is not unitary, and not time reversible We can show that the energy of the system is not conserved over time, through the same reasoning as before. The two eigenvalues of the matrix are :

$$\lambda_\pm = 1 \pm i\delta\tau$$

Which leads to divergence of the energy with the following expression :

$$\begin{aligned}H &= \frac{1}{2}\langle 0|0\rangle\left(1+\delta\tau^2\right)^n \\ &= \frac{1}{2}\langle 0|0\rangle \exp\left(n\ln\left(1+\delta\tau^2\right)\right)\end{aligned}$$

This divergence of the system can be seen in the following figure **??**

c) Verlet Algorithm & Propagator

The Verlet algorithm is a second-order algorithm, which is based on the symplectic structure of the phase space and directly derived from the splitting method. The point is to split the Hamiltonian into two parts, one depending only on the position and the other only on the impulsion.

$$H = H_q + H_p$$

With $H_q = U(q)$ and $H(p) = \frac{p^T M^{-1} p}{2}$. If we just do that it is obviously from the shadow Expansion of the Hamiltonian (REF EQ) an order one method (the Euler sympletic method). For the velvet algorithm we want that the order one term vanishes in, which leads to the following splits:

$$H = H_1 + H_2 + H_3$$

with the following possibility :

$$\begin{cases} H_1 = H_3 = \frac{1}{4}p^T M^{-1} p & | \quad H_2 = U(q) \\ H_1 = H_3 = \frac{1}{2}U(q) & | \quad H_2 = \frac{1}{2}p^T M^{-1} p \end{cases}$$

One can show that the first oder term vanishes in the shadow Hamiltonian, which defined a second order method. The first split is called the **position Verlet algorithm** , and the second the **velocity Verlet algorithm** . Let's focus on the velocity algorithm, this split is equivalent to the following change of variable :

$$\hat{\mathbf{P}} = \mathbf{P} - \frac{h}{2}\nabla U(\mathbf{q}) \tag{2.3}$$

$$\mathbf{Q} = \mathbf{q} + \frac{h}{2}\mathbf{p}^T M^{-1}\mathbf{p} \tag{2.4}$$

$$\mathbf{P} = \hat{\mathbf{P}} - \frac{h}{2}\nabla U(\mathbf{Q}) \tag{2.5}$$

This consist in a first drift $\frac{h}{2}\nabla U(\mathbf{q}$, following by a kick $\frac{h}{2}\mathbf{p}^T M^{-1}\mathbf{p}$ and a final kick. This respect the hamiltonian stucture of the system and gives the following propagation matrix :

$$\mathcal{T}(\delta\tau) = \begin{pmatrix} 1 - \frac{\delta\tau^2}{2} & \delta\tau \\ -\delta\tau\left(1 - \frac{1}{4}\delta\tau^2\right) & 1 - \frac{\delta\tau^2}{2} \end{pmatrix}$$

Here we find an unitary matrix, which conserves the pseudo energy of the system over time. Indeed using this scheme the eigenspaces are not orthogonal anymore, the true energy is then not conserved however we can still study the conserved quantities and show that :

$$\begin{aligned}\langle 0|A|0\rangle &= \langle\tau|A|\tau\rangle \\ &\Rightarrow A \equiv \mathcal{T}^\dagger A \mathcal{T} \\ &\Rightarrow A \propto \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{(1-\delta\tau^2/2)^2} \end{pmatrix} \underset{\delta\tau\to 0}{\longrightarrow} \propto H\end{aligned}$$

This can be related to the discussion on the *shadow* Hamiltonian, were we saw that the Hamiltonian describing the system in these kind of integrations was changing, due to commutator terms. Hence, the true energy is not conserved but the energy corresponding to the exact desciption of the integration system is definitely conserved.

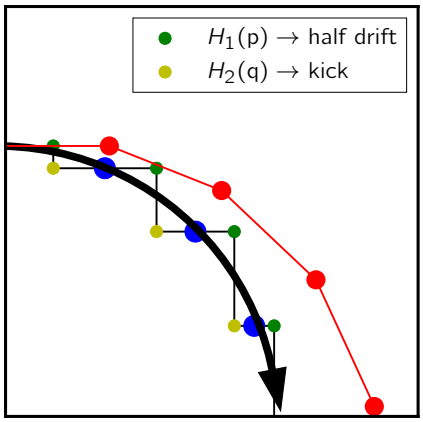

Figure 2.2 – Here we compared the construction of the flow map for the euler and the velvet algorithm. We can see that for great time steps the Euler algorithm diverges from the true flow map, while the velvet algorithm stays close to the true flow map.

This is quite relevant to notice that for periodic system the euler algorithm is definitely not stable due to the non conservation of the volume. We can also see that as a consequence of taking the tangent for each time steps as the true flow map, since it will leads us further from the trajectory in the phase space at each time step. This is why the velvet algorithm is a better choice for time integration of Hamiltonian systems.

Constant Temperature Dynamics

In molecular dynamics simulations, maintaining a constant temperature is essential for studying temperature-dependent properties, sampling thermodynamic ensembles, and ensuring accurate results. Various thermostats have been developed to control the temperature of the system, each with its own advantages and limitations. In this chapter, we will explore some common thermostats used in constant-temperature

molecular dynamics simulations and discuss their properties. In constant-temperature Molecular Dynamics, thermostats are essential to ensure that the system stays at a desired temperature, enabling accurate sampling of thermodynamic ensembles and studying temperature-dependent properties. Without a thermostat, temperature fluctuations, numerical artifacts, or deviations from the intended ensemble could lead to nonphysical results. Thermostats such as Nosé-Hoover, Langevin, and velocity rescaling provide various ways to control the temperature, depending on the specific needs of the simulation.

I. Different Ensembles

In statistical physics, an ensemble is a large collection of hypothetical copies of a system, each representing a possible state that the system can be in. Ensembles are used to describe the macroscopic properties of systems based on the statistical behavior of their microscopic components. The concept of ensembles is fundamental in statistical mechanics because it allows the connection between microscopic interactions (the behavior of individual particles) and macroscopic observables (such as temperature, pressure, and magnetization).

A. Microcanonical Ensemble

The microcanonical set is the simplest ensemble in statistical mechanics, where the system is isolated and has a fixed energy. It is described using a constant number of particles N, volume V, and energy E. In an isolated system the fundamental postulates states that the system will explore all possible microstates with the same probability. Hence we can define the density of micro-states for the microcanonical ensemble as :

$$\rho_{\text{eq}} = \frac{1}{\Omega}$$

Where Ω is the number of microstates of the system with energy E,some key properties can be derived from this definition, such as the entropy of perfect gas, thermodynamic equilibrium pressure and chemical potential properties, but we will assume that known for the reader. The Microcanonical ensemble is the one used when one simulate a physical system due to conservation laws regarding the Energy, however it is much more convenient to work with constant Temperature, for this we can introduce the canonical ensemble.

II. Canonical Ensemble

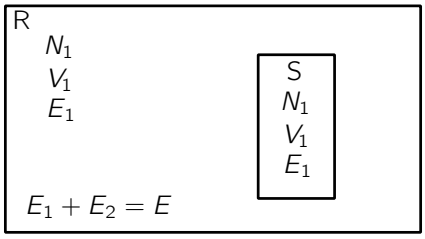

Figure 3.1 – Canonical ensemble schematic representation

In the Canonical ensemble we consider that our system is in contact with a biog reservoir, thus this two system composed a bigger isolated system. Then since the system $\mathcal{S}+\mathcal{R}$ is a microcanonical ensemble we get the following :

$$p_{\mathcal{S}} = \frac{\Omega_{\mathcal{R}}(E_{\mathcal{R}} = E - E_{\mathcal{S}})}{\Omega_{\text{tot}}}$$

Considering the reservoir at equilibrium we get :

$$\Omega_{\mathcal{R}}(E_{\mathcal{R}} = E - E_{\mathcal{S}}) = \exp\left[\frac{S_R}{k_B}(E - E_S)\right]$$

then if we develop the entropy around the mean energy of the system we get :

$$p_{\mathcal{S}} = \frac{1}{Z}\exp\left(-\frac{E_S}{k_B T_0}\right)$$

This stands for the Boltzmann-Gibbs distribution with Z defining the partition function of the canonical ensemblem and verifying the following relation :

$$Z = \sum_{\eta} \exp(-E_\eta / k_B T_0)$$

.

III. Thermostats

This huge reservoir we used in the canonical ensemble is called a thermostat and is really conveniant to dissipate external constraints apply on our system $\mathcal{S}$ while conserivng the temperature. This object can be defined in several ways from deterministic thermostats to stochastic thermostats.

A. Langvin Thermostat

The Langevin thermostat is a stochastic thermostat that introduces a friction term and a random force to the equations of motion. This thermostat mimics the effect of a heat bath on the system, providing a way to control the temperature and simulate the system's interaction with its environment. The Langevin equatiions are given by :

$$\begin{cases} 0 = \xi v(t) - kx(t) + f(t) \\ \langle f(t) f(t') \rangle = 2k_B T \xi \delta(t - t') \\ \langle f(t) \rangle = 0 \end{cases}$$

With the characteristic time $\tau = \xi / k$ and the friction coefficient ξ.