The arrow of time

Janos Polonyi
University of Strasbourg
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Contents

I. INTRODUCTION

The space and time represent different structure in non-relativistic physics. While the space coordinates of an event are constructed by the help of appropriately chosen "meter rods", the time is inferred by observing periodic motions. In addition, we need a counter, a memory, to count the number of cycles. This is a rather complicated procedure and suggests that the time and the space have actually different properties.

Such an expectation has been shattered by the advent of special relativity where the physical events are supposed to be imagined as points of the space-time, a four dimensional manifold, and labeled by one time and three space coordinates, $x^\mu = (x^0, \boldsymbol{x})$, $\mu = 0, 1, 2, 3$, $x^0 = ct$, see Fig. 1 for the world line of a particle. The Lorentz transformation, expressing a symmetry of all known

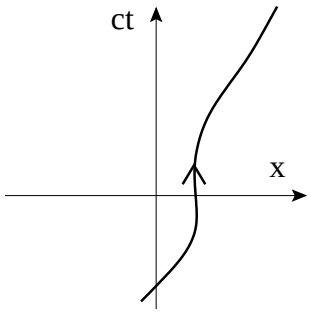


FIG. 1: The world line representation of the motion of a point particle in relativity.

interactions, mixes space and time coordinates and suggests a very close similarity between space and time. Furthermore the gravitational interaction emerges in general relativity as a feature of the geometrical of the four dimensional space-time. One tends to conclude from here relativistic physics unifies space and time.

However this is not the case, there are number of exceptions and irregularities, related to the time:

1. The invariant length square of special relativity, $s^2 = c^2t^2 - \boldsymbol{x}^2$, assigns different sign to the temporal and the spatial separations.

2. Classical, macroscopic objects can be moved in either direction in space but their time has a unique direction, rendering the physics of our body and of the world around us irreversible, as indicated on Fig. 2.

3. Time is extracted from space: Any time measuring apparatus is based on periodic motion in space. Irreversibility, the previous point, is essential here since the measurement of the time by a periodic motion requires a counter with a memory and the preservation of information assumes irreversibility. In other words, the time is directed by definition. Note that the argument is valid only in macroscopic physics.

4. The time is an inherently classical concept, it remains a c-number in quantum mechanics in contrast to the coordinates which are represented by operators.

5. The time labels the causal structure of events by distinguishing cause and effect and a causal time arrow points from the cause to the effect in time.

Once the existence of an orientation of time is accepted one may extract two time kinf of time arrows:

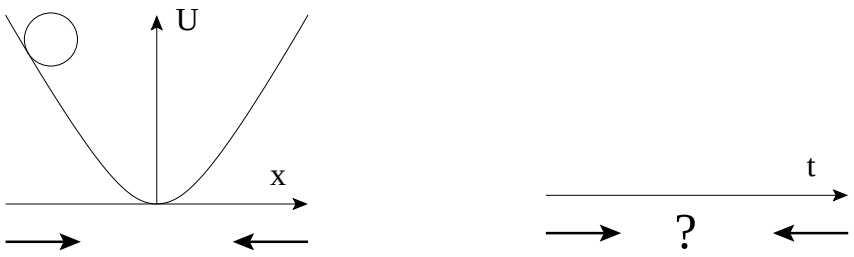


FIG. 2: The direction of the displacement in space is not unique, as opposed to the time.

1. τ_d: The dynamics distinguishes the two different orientations of the time. The usual example is irreversibility: The dynamics is stable and relaxing in the direction of the dynamical time arrow and is self-accelerating and unstable in the opposite direction. The dynamical time arrow is encoded by the time reversal invariance breaking terms of the equations of motion, e.g. Newton's friction force.

2. τ_c: The causal time arrow can be constructed by the following thought experiment. Let us consider two copies of our system which are sufficiently well separated to exclude the interactions between them. In addition we rearrange an external force, acting for $t_1 < t < t_2$ on one of them. If the systems produce different behavior exclusively for $t < t_1$ or for $t_2 < t$ then they possess a causal time arrow, $\tau_c = -1$ or $\tau_c = 1$, respectively. Hence the causal time arrow is defined by the cause-result relation.

   The causal time arrow, determined experimantelly by this procedure is implemented in our calculations by imposing the initial ($\tau_c = 1$) or the final conditions ($\tau_c = -1$) hence τ_c points away from the auxiliary conditions. One can easily construct models, defined by using both initial and final conditions, which possess no causal time arrow.

Several questions arise at this point:

- How can one recognize the direction of a dynamical time arrow experimentally? The procedure is quite simple: Make a video recording of the phenomenon in question, play it backward and check whether what one sees is a possible phenomenon or not. The time arrow exists in the latter case and points into the direction of the possible motion. For instance, the motion of a billiard ball with negligible energy loss is reversible and the sliding on a surface with friction is irreversible.

- Are there systems with no causal time arrow? This is a highly non-trivial issue since the

microscopic systems are indeterministic and the individual events possess no causal time arrow. All one knows is that the averages behave in a deterministic manner and display a causal time arrow.

- Are the causal and the dynamical time arrow identical? The different time arrows are found to be related in simple models, c.f. section III D.

- The fundamental interactions are time reversal invariant and leave the time unoriented. (To be precise one should mention that the weak interaction assigns a dynamical time arrow but that turns out to be too weakly defined to become the source of the robust direction of time, observed in macroscopic physics.) Where do the time arrows come from in a world, governed by time reversal invariant physical laws?

The main motivation of this lecture is to seek the answer to the last question. We proceed by seprating the following time arrows:

1. Electromagnetic time arrow: Imagine a person, entering in a dark room and switching on the light. When the video recording seen played backward with very fine time resolution then one notices that the room becomes dark before the person's hand reaches the electric switch. (retarded radiation field)

2. Mechanical or thermodynamical time arrow: Someone writes something on a sheet of paper with a fountain pen. The writing is a stable carrier of information because the ink diffuses into the paper. Seeing this backward in a movie one sees a bizarre, irrealistic phenomenon: the pen sucks the ink from the paper. (irreversibility)

3. Quantum time arrow: The interference in Young's double-slit experience arises from the difference of the phase of the particle's wave function when they traverse the two slits. When we monitor which slit is the particle passes then the interference disappears, the phase at the "other" slit is lost and can not be recovered. (loss of information at the quantum-classical transition)

4. Cosmological time arrow: The Big Bang, recorded by an (unidentifiable?) external witness. (cosmological initial conditions)

The time arrow problem is specially challenging and exciting because its understanding points well beyond a single chapter of physics and presses us to develop a global vision.

II. ELECTRODYNAMICS

The traditional Maxwell equations,

$$\begin{aligned} 4\pi\rho &= \boldsymbol{\nabla}\boldsymbol{E}, \\ \frac{4\pi}{c}\boldsymbol{j} &= -\frac{1}{c}\partial_t\boldsymbol{E} + \boldsymbol{\nabla}\times\boldsymbol{B}, \\ 0 &= \boldsymbol{\nabla}\boldsymbol{B}, \\ 0 &= \frac{1}{c}\partial_t\boldsymbol{B} + \boldsymbol{\nabla}\times\boldsymbol{E}, \end{aligned} \tag{1}$$

are given in terms of the electric and the magnetic fields. The first two determine the electromagnetic field induced by a given charge distribution encoded by the electric current, $j^\mu = (c\rho, \boldsymbol{j})$. The second half of the system of equations expresses the absence of magnetic charges and Faraday's induction law. This is sufficient in classical physics but we need a different description of the electromagnetic interaction in Quantum Mechanics to keep track of the interference of particle waves. The solution is the use of a vector potential, $A_\mu(x)$, to describe the electromagnetic field rather than the vectors $\boldsymbol{E}(x)$ and $\boldsymbol{B}(x)$.

The argument consists of the following steps:

1. The transformation $\psi(x) \to e^{i\chi}\psi(x)$ of the wave function is symmetry of quantum mechanics because it leaves the expectation values unchanged.

2. Such a global, space-time independent phase symmetry forces us to change the wave function in an identical manner even for space-time points, events, which are separated by space-like intervals. These events are acausal, there is no way to send information from one to the other about the needed phase change. Thus the global symmetries are in contradiction with causality. The agreement with Special Relativity is recovered by extending the phase symmetry to local gauge transformations, $\psi(x) \to e^{i\chi(x)}\psi(x)$.

3. One encounters a problem in gauge invariant quantum mechanics, namely the gauge transformation changes the momentum of a particle. In fact, we have the transformation $\boldsymbol{p}\psi = \frac{\hbar}{i}\boldsymbol{\nabla}\psi \to e^{i\chi}(\frac{\hbar}{i}\boldsymbol{\nabla}\psi + \hbar\boldsymbol{\nabla}\chi\psi) = e^{i\chi}(\boldsymbol{p}\psi + \hbar\boldsymbol{\nabla}\chi\psi)$. Were only the first term present the expectation value of momentum would remain invariant however the second term changes the expectation value.

4. To restore the invariance of the momentum, more precisely the homogeneous transformation law $\boldsymbol{p}\psi \to e^{i\chi}\boldsymbol{p}\psi$ without the disturbing inhomogeneous term, the partial derivative is replaced by the covariant derivative, $\partial_\mu\psi(x) \to D_\mu\psi(x) = [\partial_\mu - iA_\mu(x)]\psi(x)$, using the transformation rule $A_\mu(x) \to A_\mu(x) + \partial_\mu\chi(x)$ for the gauge field $A_\mu(x)$. The gauge field, $A_\mu(x) = (\phi(x), -\boldsymbol{A}(x))$, introduced in such a manner is *the* electromagnetic field.

The absence of magnetic charge suggests the definition

$$\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A} \tag{2}$$

of the magnetic field which brings Faraday's law into the form

$$0 = \boldsymbol{\nabla} \times \left(\boldsymbol{E} + \frac{1}{c} \partial_t \boldsymbol{A} \right), \tag{3}$$

suggesting $\boldsymbol{E} + \frac{1}{c}\partial_t \boldsymbol{A} = -\boldsymbol{\nabla}\phi$ or

$$\boldsymbol{E} = -\boldsymbol{\nabla}\phi - \frac{1}{c}\partial_t \boldsymbol{A}. \tag{4}$$

Note that the magnetic and electric fields, defined by eqs. (2)-(4), remain unchanged during the gauge transformation

$$\phi(x) \to \phi(x) + \frac{1}{c}\partial_t \chi(x), \quad \boldsymbol{A}(x) \to \boldsymbol{A}(x) - \boldsymbol{\nabla}\chi(x), \tag{5}$$

found for the gauge field $A^\mu = (\phi, \boldsymbol{A})$. Such a gauge invariance can be used to impose an additional gauge condition on the gauge potentials. We shall use the Lorentz gauge,

$$\frac{1}{c}\partial_t \phi + \boldsymbol{\nabla}\boldsymbol{A} = 0 \tag{6}$$

where the inhomogeneous Maxwell equations become

$$\begin{aligned} 4\pi\rho &= -\boldsymbol{\nabla}\left(\boldsymbol{\nabla}\phi + \frac{1}{c}\partial_t \boldsymbol{A} \right) = \left(\frac{1}{c^2}\partial_t^2 - \Delta \right) \phi = \Box\phi, \\ \frac{4\pi}{c}\boldsymbol{j} &= \frac{1}{c}\partial_t \left(\boldsymbol{\nabla}\phi + \frac{1}{c}\partial_t \boldsymbol{A} \right) + \boldsymbol{\nabla} \times \boldsymbol{\nabla} \times \boldsymbol{A} = \left(\frac{1}{c^2}\partial_t^2 - \Delta \right) \boldsymbol{A} = \Box \boldsymbol{A}. \end{aligned} \tag{7}$$

These wave equations can be summarized by the help of the current $j^\mu = (c\rho, \boldsymbol{j})$ as

$$\Box A^\mu = \frac{4\pi}{c} j^\mu. \tag{8}$$

A. Radiation field

We assume that the electric current arises from a charge e following the world line $x^\mu(s)$. The corresponding current is localized along the world line and satisfies the continuity equation, i.e. has the structure $j^\mu = (\rho c, \boldsymbol{j})$ where ρ and $\boldsymbol{j}$ are the charge density and the non-relativistic current, respectively. Hence it can be written in the form

$$j^\mu(x) = ec \int ds \dot{x}^\mu(s) \delta(x - x(s)). \tag{9}$$

To obtain a unique solution of eq. (8) we need some auxiliary conditions, to be imposed either at the initial or at the final time. A second order equation requires two auxiliary conditions, usually the value of the electromagnetic field and its time derivative, both taken either at the initial or at

finite time. By placing the auxiliary conditions in the distant past or future, $x^0_{\substack{in\\out}} \to \mp\infty$, where the electromagnetic field solves the homogeneous wave equation we can write the desired solution of (8) as the sum of a homogeneous and the inhomogeneous solutions, $A = A_h + A_{ih}$ in such a manner that A_{ih} and its time derivative are vanishing at the initial or final time. The homogeneous solution, appearing in the initial or final condition problem is called in our out field, A_{in} and A_{out}, respectively.

There are two ways to find the inhomogeneous solution, one either uses the retarded or advanced Green's functions, derived in appendix B, or follows a simpler, more heuristic arguemnt. The latter start with the observation that the electromagnetic field at the space-time point x must come from such a point x' which satisfies the relation $x^0 - x'^0 = \pm|\boldsymbol{x} - \boldsymbol{x}'|/c$. The choice of the sign decides whether the source of the radiation is before or after the observation, both alternative being allowed by the time reversal invariant Maxwell equations. Since the velocity of the massive charge is smaller than the speed of light there is at most one space location for each choice of the sign and x' defined in such a manner is called retarded or advanced source event for the sign + or -, respectively. Hence the free choice of the sign here defines the causal time arrow. The induced field is easy to find in a reference frame where the charge is at rest at x', it consists of a Coulomb potential without magnetic field,

$$A^\mu_{ih} = \left(\frac{e}{c|\boldsymbol{x} - \boldsymbol{x}'|}, \boldsymbol{0}\right) = \left(\pm\frac{e}{c(x^0 - x'^0)}, \boldsymbol{0}\right). \tag{10}$$

This vector potential can be rewritten in a manifestly covariant form as

$$\begin{aligned} A^\mu_{ih}(x) &= \pm e\frac{\dot{x}^\mu(s')}{(x - x')_\mu \dot{x}^\mu(s')}, \\ &= \frac{1}{c}\int d^4y \frac{\delta(x^0 - y^0 \mp |\boldsymbol{x} - \boldsymbol{y}|)j^\mu(y)}{|\boldsymbol{x} - \boldsymbol{y}|}, \\ &= \frac{1}{c}\int d^3y \frac{j^\mu(x^0 \mp |\boldsymbol{x} - \boldsymbol{y}|, \boldsymbol{y})}{|\boldsymbol{x} - \boldsymbol{y}|}, \end{aligned} \tag{11}$$

where $x^\mu(s)$ is the worldline of the charge, the invariant length s' corresonding to the event x' and the Lorentz invariant denominator is evaluated in the rest frame of the charge. The solution, given ion terms of the retarded and advanced Green's functions, $\overset{r}{D^a}(x)$,

$$\begin{aligned} A^\mu_{ih}(x) &= \frac{4\pi}{c}\int d^4y \overset{r}{D^a}(x - y)j^\mu(y), \\ &= \frac{1}{c}\int d^4y \frac{\delta(x^0 - y^0 \mp |\boldsymbol{x} - \boldsymbol{y}|)j^\mu(y)}{|\boldsymbol{x} - \boldsymbol{y}|}, \end{aligned} \tag{12}$$

is identical. This result shows clearly the choice of the initial (final) conditions leads to the the retarded (advanced) solutions and determines the causal time arrow.

B. Origin of the time arrow

The time reversal invariant Maxwell equations have two different, a retarded and an advanced solutions, neither of them preserving the time reversal symmetry, $D^{\overset{r}{a}}(x^0, \boldsymbol{x}) \neq D^{\overset{r}{a}}(-x^0, \boldsymbol{x})$ and both possess well defined causal time arrow. The coice of the initial or final conditionis leads to retarded and advanced solutions, respectively. Hence the problem of the electromagnetic time arrow consists of the following two issues:

1. We need a rule to select the linear superposition of these solutions to reproduce the observed radiation. Our daily experience shows convincingly that the retarded solution should be used and an initial condition problem should be solved.

2. We have to find the physical origin of the breaking of the time reversal invariance. On the one hand, the final conditions for the electromagnetic field are obviously unknown but on the other hand, the trivial initial conditions, $A_{in} = \partial_t A_{in} = 0$, assumed to be valid in the distant past.

Therefore the electromagnetic time arrow problem can only be solved in cosmology, by understanding the weakness of the cosmic microwave background radiation.

III. OPEN SYSTEMS

The physical system we observe is always in interaction with the rest of the Universe and the usual equations of motion, held for closed systems, are only approximate. The impact of the environment can be minimized for a short period of time but the isolation is weaken during a sufficiently long time of observation. Hence it is of greate importance in physics to describe the open, the so called effective dynamics. The main diference with the equation of motion of closed dynamics is that the latter is assumed to be local in time. in fact, a perturbation of the system generates a change in the environment whose dynamical degrees of freedom send back to the system the reaction to this original perturbation for a long while. The non-local nature of the effective equation of motion makes our intuition and mathematical tools, based on local equations, useless, for instance the stability of the motion is usually lost and Noether's theory becomes powerless. It is shown in this section the interactions with the environment always generates a causal time arrow for an open system.

The problem becomes more severe when the observed system is macroscopic:

1. The isolation of a large systems from the environment is more difficult. This difficulty is is driving force of the classical limit of large systems.

2. Avogadro's number, 6×10^{23} is quite large, the macroscopic systems possess an exceedingly large number of degrees of freedom. The resulting difficulty is addressed from the point of view of the time arrow in section IV.

A. Effective dynamics

The origin of a time arrow in a system, obeying reversible equations of motion must come from "outside", from its environment. Let us assume that the observed system and its environment are described by the coordinates x and y, respectively, subject of a local, reversible and stable equations of motion,

$$\ddot{x}(t) = F(x(t), y(t)), \quad \ddot{y}(t) = G(x(t), y(t)), \tag{13}$$

supplied by the auxiliary conditions,

$$x(t_a) = x_a, \quad \dot{x}(t_a) = v_a, \quad y(t_a) = y_a, \quad \dot{y}(t_a) = u_a. \tag{14}$$

The environment coordinate is not observed hence it has to be eliminated from the equation of motion of the observed system. This is achieved by solving the environment equation of motion and inserting the solution, $y[t, x, y_a, u_a, t_a]$, back into the system equation of motion. The result is a non-local equation of motion,

$$\ddot{x}(t) = F(x(t), y[t, x, y_a, u_a, t_a]), \tag{15}$$

which defines an effective dynamics. The word "effective" is a synonym of "open" and indicates the presence of an environment, taken into account by the involved, non-local terms of the equation of motion, usually approximated by a local expressions, obtained within the framework of the expansion in the time derivative.

A physical laws, expressed as a differential equation, are incomplete and acquire predictive power only after providing the necessary auxiliary conditions which render their solution unique. The symmetry with respect to time reversal, the absence of time arrow, refers to the equations only and the auxiliary conditions break the formal time reversal symmetry of the solution in a trivial manner. The distinguishing feature of effective equations of open dynamics is that presence of the environment auxiliary conditions, y_a, u_a and t_a in the equations of motion.

Since the initial and the final auxiliary conditions differ the environment auxiliary conditions always break the time reversal invariance of the equation of motion and a system time arrow is generated. Suppose that we make a video recording of the dynamics of the system. Though we see the environment in the recording our experience about the direction of the time of the effective dynamics allows us to recognize that a scene, seen on the backward played video recording is unusual in what the system and the environment have opposite direction of their time.

It will be shown that an open system develops an oriented time by borrowing the time arrow from an environment. Such a transmutation of the time arrow is reminiscent of the electromagnetic time arrow except that it is the environment rather than the systems own initial condition is concerned.

B. Harmonic toy model

A simple toy model to study the transfer of the time arrow consist of an observed harmonic oscillator which is coupled to N unobserved oscillators in a linear manner. A typical example is an atom where the small deformations of the electronic structure can be approximated by a harmonic oscillator, coupled to the electromagnetic field. The Lagrangian is

$$\begin{aligned} L &= \frac{m}{2}\dot{x}^2 - \frac{m\omega_0^2}{2}x^2 - jx + \sum_n \left(\frac{m}{2}\dot{y}_n^2 - \frac{m\omega_n^2}{2}y_n^2 - g_n x y_n\right) \\ &= \frac{m}{2}\dot{x}^2 + \left(\frac{m\omega_0^2}{2} - \sum_n \frac{g_n^2}{2m\omega_n^2}\right)x^2 - jx + \sum_n \left[\frac{m}{2}\dot{y}_n^2 - \frac{m\omega_n^2}{2}\left(y_n + \frac{g_n x}{m\omega_n^2}\right)^2\right], \end{aligned} \tag{16}$$

where the external source, $j(t)$, is introduced to diagnose the system and the inequality, $m\omega_0^2 > \sum_n \frac{g_n^2}{m\omega_n^2}$, is assumed to stabilize the dynamics. The initial conditions, $x_i = v_i = 0$ are imposed at $t_i \to -\infty$ for the observed system and either initial or final conditions are used for the environment, $y_{ni} = u_{ni} = 0$ with $t_i = -\infty$ or $y_{nf} = u_{nf} = 0$ with $t_f = \infty$, respectively.

The environment equations of motion, $m\ddot{y}_n = -m\omega_n^2 y_n - g_n x$, written for the Fourier transform,

$$x(\omega) = \int dt e^{i\omega t} x(t), \tag{17}$$

in the frequency space as

$$m\omega^2 y_n(\omega) = m\omega_n^2 y_n(\omega) + g_n x(\omega), \tag{18}$$

can easily be solved,

$$y_n(\omega) = \frac{g_n x(\omega)}{m(\omega^2 - \omega_n^2)} = \tilde{D}_n(\omega) g_n x(\omega). \tag{19}$$

The environment Green's function,

$$\tilde{D}_n(\omega) = \frac{1}{m[(\omega + i\epsilon_e)^2 - \omega_n^2]} \tag{20}$$

is used with $\epsilon_e > 0$ and $\epsilon_e < 0$, for initial and final conditions, respectively. The insertion of this trajectory into the equation of motion of the system coordinate yields the effective equation of motion,

$$j(\omega) = \{m[(\omega + i\epsilon_s)^2 - \omega_0^2] - \tilde{\Sigma}(\omega)\}x(\omega) = \tilde{D}_{eff}^{-1}x(\omega), \tag{21}$$

where $\epsilon_s > 0$ and the self energy,

$$\tilde{\Sigma}(\omega) = \sum_n g_n^2 D_n(\omega) = \sum_n \frac{g_n^2}{m}\frac{1}{(\omega + i\epsilon_e)^2 - \omega_n^2}, \tag{22}$$

is used to define the effective Green's function,

$$\tilde{D}_{eff}(\omega) = \frac{1}{m[(\omega + i\epsilon_s)^2 - \omega_0^2] - \tilde{\Sigma}(\omega)}. \tag{23}$$

The system trajectory, corresponding to a given external source satisfies the effective equation of motion,

$$\tilde{D}_{eff}^{-1}x(\omega) = m\left[(\omega + i\epsilon_s)^2 - \omega_0^2 - \sum_n \frac{g_n^2}{m}\frac{1}{(\omega + i\epsilon_e)^2 - \omega_n^2}\right]x(\omega) = j(\omega), \tag{24}$$

which is non-local in time because it contains arbitrarely high powers of $\omega \sim i\partial_t$.

C. Spectral function

A realistic environment is large and the limit $N \to \infty$ can conveniently be parameterized by the help of the spectral function,

$$\rho(\Omega) = \sum_n \frac{g_n^2}{2m\omega_n}\delta(\omega_n - \Omega), \tag{25}$$

which allows us to write

$$\tilde{\Sigma}(\omega) = \int d\Omega \frac{2\rho(\Omega)\Omega}{(\omega + i\epsilon_e)^2 - \Omega^2}. \tag{26}$$

A simple, non-trivial phenomenological ansatz is Drude's expression,

$$\rho(\Omega) = \Theta(\Omega)\frac{g^2\Omega}{m\Omega_D(\Omega_D^2 + \Omega^2)}, \tag{27}$$

yielding

$$\begin{aligned}\tilde{\Sigma}(\omega) &= \frac{g^2}{m\Omega_D}\int d\Omega\Theta(\Omega)\frac{\Omega}{\Omega_D^2+\Omega^2}\frac{2\Omega}{(\omega+i\epsilon_e)^2-\Omega^2}\\ &= -\frac{g^2}{m\Omega_D}\int d\Omega\frac{\Omega^2}{(\Omega+i\Omega_D)(\Omega-i\Omega_D)(\Omega-\omega-i\epsilon_e)(\Omega+\omega+i\epsilon_e)}\\ &= -\frac{g^2}{m\Omega_D}2\pi i\left[\frac{\Omega_D^2}{2i\Omega_D(\omega^2+\Omega_D^2)}+\mathrm{sign}(\epsilon_e)\frac{\omega^2}{(\omega^2+\Omega_D^2)2(\omega+i\epsilon_e)}\right]\\ &= -\frac{g^2\pi}{m\Omega_D}\frac{\Omega_D+i\mathrm{sign}(\epsilon_e)\omega}{\omega^2+\Omega_D^2} = -\frac{\pi g^2}{m\Omega_D(\Omega_D-i\mathrm{sign}(\epsilon_e)\omega)}\end{aligned} \tag{28}$$

and

$$\tilde{D}_{eff}(\omega) = \frac{1}{m[(\omega+i\epsilon_s)^2-\omega_0^2]+\frac{\pi g^2}{m\Omega_D(\Omega_D-i\mathrm{sign}(\epsilon_e)\omega)}}. \tag{29}$$

The choice of the system auxiliary conditions, encoded by $\mathrm{sign}(\epsilon_s)$, is irrelevant owing to the finiteness of $\mathrm{Im}\tilde{\Sigma}$,

$$\tilde{D}_{eff}(\omega) = \frac{1}{m(\omega^2-\omega_0^2)+\frac{\pi g^2}{m\Omega_D(\Omega_D-i\mathrm{sign}(\epsilon_e)\omega)}}. \tag{30}$$

The effective equation of motion,

$$\tilde{D}_{eff}^{r-1}x(\omega) = m\left[\omega^2-\omega_0^2+\frac{\pi g^2}{m^2\Omega_D(\Omega_D-i\mathrm{sign}(\epsilon_e)\omega)}\right]x(\omega) = j(\omega), \tag{31}$$

reduces to

$$m[(\omega+i\epsilon_s)^2-\omega_{eff}^2+i\mathrm{sign}(\epsilon_e)\nu\omega]x(\omega) = j(\omega), \tag{32}$$

for slow motion, $\omega\to 0$, containing the effective parameters m_{eff} and ω_{eff}, defined by the $\mathcal{O}\left(\omega^0\right)$ and the $\mathcal{O}\left(\omega^2\right)$ part of the equation of motion,

$$\begin{aligned}m_{eff}\omega_{eff}^2 &= m\omega_0^2-\frac{\pi g^2}{m^2\Omega_D^2},\\ m_{eff} &= m-\frac{\pi g^2}{m^2\Omega_D^4},\end{aligned} \tag{33}$$

and Newton's friction constant, $\nu=\frac{\pi g^2}{m^2\Omega_D^3}$. The real time form,

$$\ddot{x}(t) = -\omega_{eff}^2x(t)-\mathrm{sign}(\epsilon_e)\nu\dot{x}(t)-j(t), \tag{34}$$

shows that infinitely many oscillator in the environment, distributed with a spectral function $\rho(\Omega)=\mathcal{O}(\Omega)$, generate dissipative friction force which makes the effective dynamics stable in the direction of the environment time arrow.

Note an imporant difference between the self energy given for discrete spectrum (22) and in case of the Drude model (28). While the flipping of $\mathrm{sign}(\epsilon_e)$ influences the former in an infinitesimal manner, similar to the change of $\mathrm{sign}(\epsilon_s)$ the change of the environment time arrow generates a finite change in the latter case for $\omega \neq 0$. The dissipation, encoded by the dissipative forces, represents an increased sensitivity of the effective dynamics on the environment time arrow. This suggests a formal similarity between phase transitions, spontaneous symmetry breaking in particular, and the generation of the system time arrow by a dissipative environment.

D. Causal time arrow

Let us start with the case of discrete spectrum. The ϵ-independent part of the poles of the Green's functions define the normal mode spectrum of our harmonic model.

- $\mathrm{sign}(\epsilon_s) = \mathrm{sign}(\epsilon_e)$: The potential energy in the second line of eqs. (16) is a positive quadratic form hence the normal mode spectrum is real. As a result, the zeros of $\tilde{D}^{-1}_{eff}(\omega)$ are in the appropriate half plane of the complex frequency and the effective dynamics is causal, c.f. Figs. 3 (a) and (b) where the system self-interaction is retarded and advanced, respectively.

- $\mathrm{sign}(\epsilon_s) = -\mathrm{sign}(\epsilon_e)$: There are poles on both complex frequency half planes and the self-interaction has no causal time arrow. In fact, the system influences the environment in the direction, set by the environment auxiliary conditions however the feed back to the system influences the system trajectory both before and after t_s in Figs. 3 (c) and (d).

It is worthwhile keeping in mind that there is another way acausality may arise in a formal calculation. Let us consider a causal but unstable dynamics which produces self accelerating, runaway trajectories. In the calculation of the Green's function by means of the residue theorem it is tacitly assumed that the trajectory is bounded, in agreement with the original assumption about the stability of the full dynamics, including the system and the environment. A pole, appearing on the "wrong" half plane would give an unacceptable, exponentially increasing runaway trajectory. To suppress it, we use the corresponding residuum for the "other" sign of the time variable, resulting in acausal Green's functions.

An environment with continuous spectrum produces a more significant effect, it overwrites the choice of the system initial conditions since ϵ_s drops out from the effective Green's function (32). The distinguishing feature of dissipative forces is that they pass the environment time arrow to the

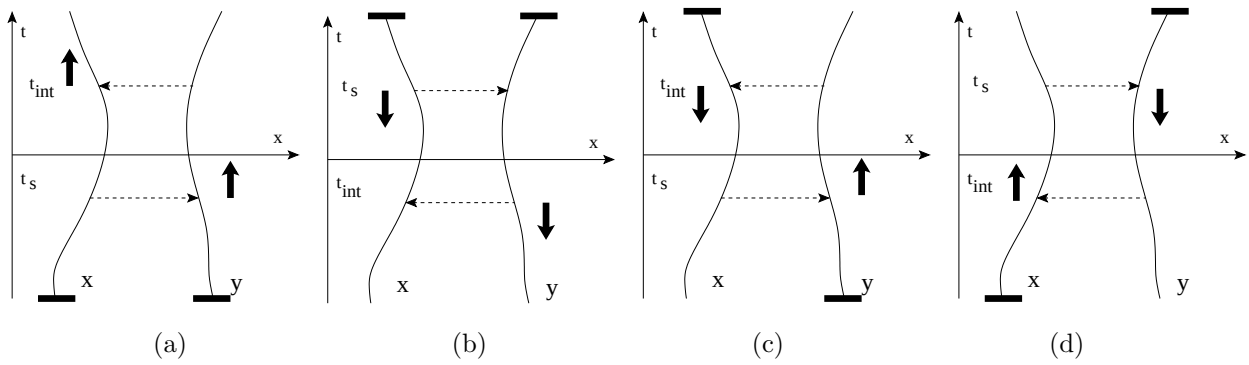


FIG. 3: The causal structure of the self interaction of the observed system, mediated by an environment with discrete spectrum. A perturbation of the system coordinate, x, is made at time t_s and the instantaneous system-environment interaction (dashed horizontal line, pointing to right) makes the environment trajectory, $y(t)$, changed in time in the direction of the environment causal time arrow (vertical arrow at right) makes the system trajectory, $x(t)$, changed in time in the direction of the system causal time arrow (vertical arrow at left). The auxiliary conditions are imposed at the initial or final time, denoted by short, fat horizontal lines. (a): $\epsilon_s >, \epsilon_e > 0$, (b): $\epsilon_s, \epsilon_e < 0$, (c): $\epsilon_s < 0$, $\epsilon_e > 0$, (d): $\epsilon_s > 0$, $\epsilon_e > 0$.

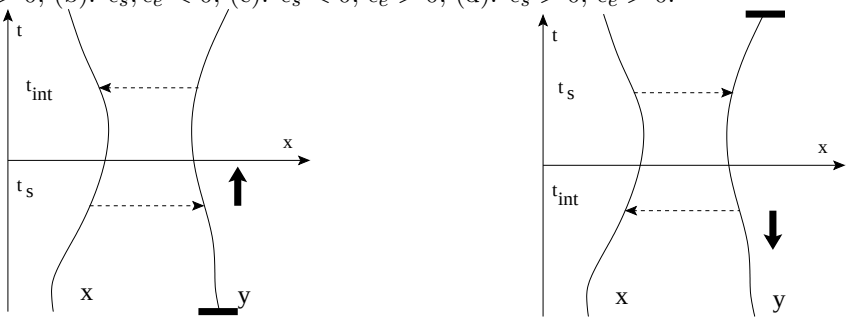


FIG. 4: The causal structure of the self interaction of a dissipative effective dynamics. The notation is the same as in Fig. 3 except the system auxiliary conditions are left out, they are "forgotten" and become obsolete during the time evolution. (a): $\epsilon_e > 0$, (b): $\epsilon_e < 0$.

system. As a result the effective system dynamics is causal and stable only in the direction of the environment time arrow as shown on Figs. 4, c.f. eq. (**??**).

E. Broken time reversal invariance and irreversibility

The breakdown of the time reversal invariance does not imply irreversibility, i.e. dissipative forces. In fact, dissipation, an unavoidable energy loss to the environment, appears only if one looses sight of the degree of freedom which absorbs the energy. The conserved total energy of the

model,

$$H = \frac{m}{2}\dot{x}^2 + \frac{m\omega_0^2}{2}x^2 + \sum_n \left(\frac{m}{2}\dot{y}_n^2 + \frac{m\omega_n^2}{2}y_n^2 + g_n x y_n \right), \tag{35}$$

can be expressed in terms of the system coordinate,

$$\begin{aligned} H(t) &= \frac{m}{2}\dot{x}^2(t) + \frac{m\omega_0^2}{2}x^2(t) + \sum_n g_n^2 \Bigg[\frac{m}{2}\left(\int dt' \partial_t D_n^r(t-t')x(t') \right)^2 \\ &\quad + \frac{m\omega_n^2}{2}\left(\int dt' D_n^r(t-t')x(t') \right)^2 + x(t)\int dt' D_n^r(t-t')x(t') \Bigg] \\ &= \frac{m}{2}\dot{x}^2(t) + \frac{m\omega_0^2}{2}x^2(t) + \sum_n g_n^2 \Bigg\{ [x(t)\int dt' D_n^r(t-t')x(t') \\ &\quad + \frac{m}{2}\int dt' dt'' x(t')[\partial_t D_n^r(t-t')\partial_t D_n^r(t-t'') + \omega_n^2 D_n^r(t-t')D_n^r(t-t'')]x(t'') \Bigg\} \\ &= \frac{m}{2}\dot{x}^2(t) + \frac{m\omega_0^2}{2}x^2(t) + \sum_n \frac{g_n^2}{m}\Bigg[-x(t)\int_{-\infty}^{t} dt' \frac{\sin\omega_n(t-t')}{\omega_n}x(t') \\ &\quad + \frac{1}{2}\int_{-\infty}^{t} dt' dt'' x(t')[\cos\omega_n(t-t')\cos\omega_n(t-t'') + \sin\omega_n(t-t')\sin\omega_n(t-t'')]x(t'') \Bigg]. \end{aligned} \tag{36}$$

The relevant lesson of this rather complicated expression is that we recognise the conserved nature of the effective dynamics only if each contribution to the sum can be reconstructed by observing the system trajectory, $x(t)$.

The time t_{obs} of an observation of a periodic motion, $x(t)$, and the precision $\delta\omega$ of the prediction of the frequency of the motion satisfy an uncertainty principle, $t_{obs}\Delta\omega = a$, where the value of a depends on the way the frequency is inferred from the observation. In fact, the prediction of the frequency from the measured values of $x(t)$ is the result of some kind of fitting procedure which becomes more precise if more period lengths are covered by the fit. In the absence of any other relevant time scale in the problem $\Delta\omega \sim 1/t_{obs}$.

Let us asume that the spectrum is discrete and the normal frequencies are separated at least by $\Delta\omega > 0$. The all spectrum line of $x(t)$ can be isolated and properly resolved by observing the system in time $t_{obs} > 1/\Delta\omega$. Hence the conserved nature of the effective dynamics can be established by a long enough observation. The is not the case anymore if the normal mode spectrum possesses a condensation point since an arbitrarely long observation is still missing infinitely many environment modes. If the condensation point is at vanishing frequency then the divergent heat capacity of a soft environment in the thermodynamical limit generates dissipative forces.

We see that infinite systems may display features which are unimaginable in the finite case: The use of dissipative forces provides an approximation which becomes excellent for large system. We need extremely long observation to discover the conserved dynamics for a macroscopic body

due to the largeness of Avogadro's number. This is a formal similarity between the dissipation as a spontaneously broken time reversal symmetry and the phase transitions, corresponding to the spontaneous breakdown of symmetries, both symmetry breaking being a good approximation for finite time observations. The non-dynamical, static diagnose of spontaneous symmetry breaking, say the the singular dependence of the magnetization on the weak external magnetic field in the case of ferromagnetism, can be paralleled with the dependence on sign(ϵ_e), discussed in section III C.

IV. THERMODYNAMICS

To deal with point 1., mentioned at the beginning of section III, we select few important, collective degrees of freedom, the thermodynamical variables, which we control. Rather than following a detailed, mechanical derivation of the equation of motion for these variables one follows another argument, based on information. The starting point, namely that the thermodynamical variables represent a partial information about the macroscopic system, is rather unusual from the point of view of the dynamical laws. Furthermore we assume that such a partial information is sufficient as long as we restrict our interest to very slow, quasi equilibrium processes where the system does not leave the (quasi)equilibrium state. The direction of time of an infinitely slow process is the provided by reproductibility: The observed dynamics of the thermodynamical variables can be reproduced in different experiments. If the monitored variables contain enough information to establish reproducible laws then the thermodynamical time arrow reflects the degradation of the partial information about the initial state.

A. Controlled and uncontrolled channels

The feature 2. of Section III leads to information loss, forcing us to accept a probabilistic treatment of the thermodynamical variables. Furthermore, it is advantageous to split the system-environment interaction channels into controllable and uncontrollable subsets, the latter being responsible of the statistical fluctuations. Statistical mechanics consists of the masterful combination of microscopic and phenomenological considerations about the thermodynamical variables, made possible by the narrowing of the probability distributions around their peaks in the thermodynamical limit. The result is thermodynamics, a set of deterministic equations for the location of the peaks.

Consider the average energy as an example. It can be written in the form of an expectation value,

$$E = \langle H \rangle = \sum_n p_n E_n \tag{37}$$

whose change in an infinitesimal time,

$$\delta E = \delta Q + \delta W, \tag{38}$$

is the sum of two terms. The first,

$$\delta W = \sum_n p_n \delta E_n, \tag{39}$$

is due to the shift of the energy levels. The system is under control and the change of its energy spectrum indicates that some controllable work have been performed by the system. The second,

$$\delta Q = \sum_n \delta p_n E_n, \tag{40}$$

denotes the energy received by the uncontrollable channels from the unobserved environment and is called heat. One recognizes in (38) the first law of thermodynamics.

The second law of thermodynamics has several equivalent versions. Kelvin stated that we can not convert heat into work without loss, Clausius showed that we can not transfer heat from the colder to the warmer environment without loss. Another reasoning implies his entropy, a state function, the sum of the heat exchange weighted by the inverse absolute temperature along a reversible path over equilibrium states,

$$S_{th} = \int \frac{\delta Q}{T}, \tag{41}$$

expressed in units $k_B = 1$. It follows form his arguments that the entropy changes during the evolution from state A to state B by respecting the inequality,

$$\int_A^B \frac{\delta Q}{T} \leq S_{th}(B) - S_{th}(A), \tag{42}$$

if the temperature is well defined during the process, an immediate result being that the entropy does not decrease in a thermally isolated system (in the average). The thermodynamical time arrow appears at this point and one wonders how can this happen if the underlying microscopical equations of motion are time reversal invariant.

B. Entropy of a closed system

There have been two other proposals for entropy, beyond the thermodynamical entropy, (41), Boltzmann's expression,

$$S_B = \ln \frac{\Omega}{\Omega_0}, \tag{43}$$

where Ω and Ω_0 denote the available phase space volume and the volume of a reference unit element, respectively and Gibbs' form,

$$S_G = -\int d^{3N}pd^{3N}qp(\boldsymbol{p},\boldsymbol{q}) \ln p(\boldsymbol{p},\boldsymbol{q}), \tag{44}$$

where $p(\boldsymbol{p},\boldsymbol{q})$ stands for the probability density of the classical system in the phase space. A specially troubling issue here, realized by Ehrenfest, is that these two entropies are conserved in a closed system owing to Liouville's theorem, c.f. appendix C. How can the entropy (43) and (44) of an isolated system increase?

The answer comes with a slightly new point of view of the ensembles of statistical physics. The original motivation of the statistical ensembles is ergodicity, the assumption that the measured, long time averages are equivalent with the ensemble averages. However we have a single, isolated physical system and we would like to find the origin of the entropy production without referring to an average over a formal ensemble. For that end we define the micro and the macro states: A micro state is a point in the phase space, it denotes a fully identified state of our system, including all information. The macro state, defined by the set of thermodynamical variables, Φ, represents our partial information about the system and is realized by $\Sigma(\Phi)$, the set of micro states, compatible with Φ. The thermodynamical entropy corresponds to Boltzmann's entropy of macro state, $S_{th}(\Phi) = \ln \Omega(\Sigma(\Phi))/\Omega_0$. The thermodynamical potentials should possess enough control over the micro state to lead to well defined thermodynamical laws, i.e. to generate closed equations. If we retain more than the necessary variables then a set of equations of states introduces a constraint among them. In the case of sufficient control over the micro states the dynamics of the thermodynamical variables is well defined and reproducible. This latter means that different experiments, using different micros states, discover the same time evolution of the macro states. It will be shown that the reproductibility of the thermodynamical laws makes the entropies (43) and (44), constructed for the macro states, non-decreasing in time.

C. Entropy and information

We now revisit the introduction of the ensembles in statistical physics to find the origin of their probability distribution. The probability appears in the usual treatment due to our inability to control the microscopic interaction channels and is usually associated to physical fluctuations. We adopt here another point of view, assuming that the probability is a formal device to express our lack of information about a complicated macroscopic system and define the entropy as the upper limit of the missing information. It is explained briefly in appendix D that one can arrive in this manner at a constructive definition of the probability distribution and the entropies (43) and (44).

The Gibbs entropy is obviously equivalent with the entropy, found by maximizing the missing information, (D23). Its equivalence with the Boltzmann entropy follows from the asymptotic equipartition theorem of information theory. This theorem applies for distributions which peak with width $\mathcal{O}(1/\sqrt{N})$ in the thermodynamical limit and for constraints which converge in the same limit. Let define the phase-space region, $\Sigma(\Phi,\epsilon)$, by requiring that the system is within this volume with probability $1-\epsilon$,

$$\int_{\Sigma(\Phi)} d^{3N}pd^{3N}qp(\boldsymbol{p},\boldsymbol{q}) = 1-\epsilon \tag{45}$$

and the probability is constant on its boundary, $p(\partial\Sigma)$ =const. The theorem states that the phase-space volume,

$$\Omega_N(\Sigma(\Phi),\epsilon) = \int_{\Sigma(\Phi)} d^{3N}pd^{3N}q, \tag{46}$$

approaches the Gibbs entropy in the thermodynamical limit,

$$\lim_{N\to\infty} \frac{\ln \frac{\Omega_N(\Sigma(\Phi),\epsilon)}{\Omega_0}}{N} = -\int d^{3N}pd^{3N}qp(\boldsymbol{p},\boldsymbol{q})\ln p(\boldsymbol{p},\boldsymbol{q}), \tag{47}$$

independently of the choice of $0<\epsilon<1$ and $\Omega_0>0$.

D. Second law and reproductibility

Let us first assume that our system is in equilibrium with its environment at the time t and this equilibrium state can be characterized by the thermodynamical variables, Φ. After that we isolate the system from its environment and bring it into another equilibrium state Φ' at time t' in a reproducible manner, i.e. any other measurement, based on a different initial micro state representative of the initial macro state, produces the same set of final thermodynamical

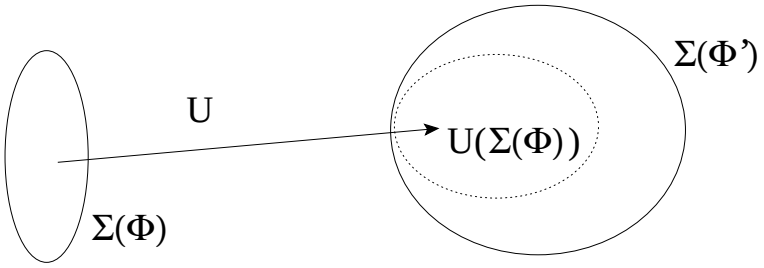


FIG. 5: The second law of thermodynamics: phase space volume of a macro state can not decrease during reproducible changes $\Phi_i \to \Phi_f$ of the thermodynamic variables.

variables. To phrase this in a mathematical statement we introduce the time evolution map, $U_{t',t} : \mathbb{R}^{6N} \to \mathbb{R}^{6N}$ for the micro states by the definition, $U_{t',t}(x(t), p(t)) = (x(t'), p(t'))$, where the trajectory $(x(t), p(t))$ is generated by the full set of microscopic equations of motion with couplings to the environment ignored. Reproductibility is the inclusion

$$U_{t_f,t_i}(\Sigma(\Phi_i)) \subset \Sigma(\Phi_f), \tag{48}$$

where $U(\Sigma)$ denotes the image of the phase space region Σ after the time evolution. According to Liouville's theorem

$$\Omega(\Sigma(\Phi_f)) = \Omega(U_{t_f,t_i}(\Sigma(\Phi_i))) \tag{49}$$

and the inequality

$$\Omega(\Sigma(\Phi_i)) \leq \Omega(\Sigma(\Phi_f)) \tag{50}$$

follows. By taking its logarithm we arrive at the second law,

$$S_{th}(\Phi_i) = \ln \frac{\Omega(\Sigma(\Phi_i))}{\Omega_0} \leq \ln \frac{\Omega(\Sigma(\Phi_f))}{\Omega_0} = S_{th}(\Phi_f). \tag{51}$$

The inequalities (48) and (51) become equality for reversible reproducible processes.

One might think that the second law of thermodynamics, applied to isolated systems, implies a breakdown of the time inversion invariance. But this interpretation is incorrect on the following counts:

1. The closed system retains its time reversal dynamics and the impression of irreversibility comes rather from our inability to possess all information. What makes the entropy non-decreasing is the loss of information about the non-thermodynamical variables. As soon as we possess all information Φ identifies the system in a unique manner and $\Omega(\Sigma(\Phi)) = (2\pi\hbar)^{3N} = \Omega_0$ becomes a constant of motion.

2. The argument about the non-decreasing of the entropy works in reversed time, too. Once the final state is specified and the time evolution is used to "predict" the corresponding initial state then the entropy is non-increasing in the time which flows backward. The time evolution in phase space preserves the time reversal invariance, it is our partial information about the system, used to designate the macro states, becomes obsolete only.

3. The construction of (equilibrium) thermodynamics, the dynamics of the thermodynamical variables, is reminiscent of the goal of an effective theory, discussed in section III, except that we are dealing equilibrium states and we ask whether certain transitions are taking place or not rather than the detailed time evolution of the observed system. The role of the observed system is played by the thermodynamical variables and the environment is replaced by the manifold of micro states within a given macro state, the missing information. The lack of the detailed equations of motion prevents us to control the status of the time reversal invariance.

The microscopic origin of the thermodynamical time arrow, the strict inequality in the second law of thermodynamics, can be found by restoring the coupling to the environment and a more careful treatment of the open dynamics, as in section III B. It turns out that Liouville's theorem is violated by the dissipative forces in such a manner that the phase space is strictly decreasing in time. Such a focusing in the phase space makes the inclusion strict in eq. (48), i.e. $U_{t_f,t_i}(\Sigma(\Phi_i))$ is strictly smaller than $\Sigma(\Phi_f)$. This can be understood by recalling that dissipative forces usually render the initial conditions irrelevant, the system approaches a relaxed state except some extreme initial conditions. Hence $U_{t_f,t_i}(\Sigma(\Phi_i))$ shrinks compared to $\Sigma(\Phi_f)$, defined at the same time as any other macro state, at t_i.

It is finally instructive to comment the need of entropy beyond the energy. The energy is not directly measurable and its importance stems from its conservation. When we intend to perform certain task by an engine then we want to send it onto a certain trajectory in the phase space. The energy is a useful quantity because it characterizes the available phase space. When we say that we give some energy to the system then we give a certain "push" in such a manner that it ends up on the desired phase space trajectory. The complications start in the thermodynamical or the statistical description when we do not wish to follow the complete dynamics in a detailed manner but we still want to keep some control over the phase space. The exchanged energy is split into two parts, corresponding to the controlled and the uncontrolled components, c.f. eq. (38) and the entropy characterizes the latter.

The thermodynamical equation, (41), can be obtained by the help of Shannon's entropy,

$$\begin{aligned} \delta S &= \delta(-\sum_n p_n \ln p_n) \\ &= -\sum_n (\delta p_n) \ln p_n \\ &= \frac{1}{T}\sum_n E_n \delta p_n \\ &= \frac{\delta Q}{T} \end{aligned} \tag{52}$$

where the relation $\sum_n \delta p_m = 1$ was used in the second equation, the canonical probability distribution (D20) is used in the second third equation and finally, the last line follows from Eq. (40). This equation, written in the form,

$$\frac{\delta Q}{T} = d \ln \Omega = \frac{d\Omega}{\Omega}, \tag{53}$$

shows that the relative change of the accessible phase is to be compared with the amount of the uncontrolled energy exchange, the exchange factor being an intensive variable, the temperature, a measure of the efficiency of the phase-space injection by an external intervention. A given amount of energy yields more gain in relative phase space at lower temperature when the energy comes in an ordered manner. Energy, injected in a disordered fashion is less efficient to enlarge the phase space due to the cancellations among the uncontrolled microscopic processes.

One can finally see a more physical definition of information: The information, missed in the environment and reflected in the entropy of the system, is the uncontrolled energy exchange, weighted by the inverse temperature. A system-environment interaction, representing a given uncontrolled energy exchange, can be traced more and more precisely (can be described by answering more and more questions about the environment) when the environment is more ordered, stronger correlated with the system. Since the environment is infinite the information diverges in the zero temperature limit.

V. QUANTUM MECHANICS

The electrodynamical, the mechanical and the thermodynamical time arrows show the importance of the environment in establishing a direction for the time. The environment plays a central role in another part of physics, in quantum mechanics, where it generates the quantum mechanical time arrow. A microscopic system can in principle be isolated and in that case the well known

rules of quantum mechanics apply. A system of a large number of particles develops dense excitation spectrum which makes the weak interactions with the environment important. In fact, a small energy exchange with the environment may lead to an excitation, a jump of the system from a stationary state of the system Hamiltonian to another, orthogonal state. The resulting strong coupling to the environment, arising in such a manner, is the driving force of the classical limit, the emergence of the classical world.

Any phenomenon, let it be microscopic or macroscopic, consists of microscopic, elementary events. A macroscopic phenomena starts with a microscopic one which growth until it reaches the macroscopic scales. There is an interesting state in this amplification process, when the size of the phenomenon reaches the quantum-classical transition scale, typically in the order of magnitude of the Bohr radius. The piercing of the quantum-classical border, when the indeterministic quantum fluctuations give rise deterministic events, is accompanied by a short living irreversible phase. The quantum mechanics time arrow appears at this moment. This process is followed as a sequence of three consecutive steps in a measurement process.

The full, closed system consists of a microscopic degree of freedom, to be measured, the measuring apparatus of an observable A of this degree of freedom and the environment. The states of these subsystems belong to the linear spaces, $\mathcal{H}_s$, $\mathcal{H}_A$, and $\mathcal{H}_e$, listed in the same order. The Hamiltonian, $H = H_0 + H_i$, is written as the sum of the subsystem Hamiltonians, $H_0 = H_s + H_A + H_e$ and the interaction terms, $H_i = H_{sA} + H_{Ae}$, where the indices indicate the interacting subsystems, and the time evolution is generated by the unitary operator $U_m = e^{-\frac{i}{\hbar}Ht_m}$ where t_m is the time needed to perform the measurement. We shall use the orthonormal bases $|\phi_k\rangle \in \mathcal{H}_s$, $|\chi_\ell\rangle \in \mathcal{H}_A$, and $|\eta_m\rangle \in \mathcal{H}_s$.

The role of the apparatus is to make the state of the microscopic system "visible", i.e. to establish a correlation between the microscopic system and the apparatus. The Hamiltonian H_A governs a macroscopic, collective degree of freedom of the measuring apparatus which displays the result of the measurement and the remaining large number of microscopic degrees of freedom of the apparatus belongs to H_e. Hence the linear space $\mathcal{H}_s \otimes \mathcal{H}_A$ describes a system of two degrees of freedom, a microscopic and a macroscopic one. In the case of measuring the current of a microscopic wire in a nanophysical experiment the microscopic system is the electric charge, moving in the wire, the apparatus consists of the needle of a current meter and the environment contains the remaining degrees of freedom of the current meter and the air molecules in the room.

A. Pre-measurement

We assume that the measurement process is sufficiently fast to treat the first step of the interaction between the microscopic system and the apparatus by ignoring the environment. The corresponding Hamiltonian, is $H_m = H_s + H_A + H_{sA}$, drives the initial state, just before the measurement, $|\phi_{k_i}\rangle \otimes |\chi_{\ell_i}\rangle$, into

$$e^{-\frac{i}{\hbar}H_m t_m}|\phi_{k_i}\rangle \otimes |\chi_{\ell_i}\rangle = \sum_{k\ell} c^{k\ell}_{k_i\ell_i}|\phi_k\rangle \otimes |\chi_\ell\rangle, \tag{54}$$

after the measurement. The initial and the final states are fundamentally different, they are factorisable and entangled, respectively. The entanglement is generated by the system-apparatus interaction, the right hand side being a factorisable state if $H_{sA} = 0$. The important lesson of this remark is that a factorisable state becomes entangled by the interactions between the subsystems. This entanglement, the first appearance of the microscopic system-measurement apparatus correlation, is called pre-measurement.

The linearity of the time evolution operator, U_m, assures that an arbitrary initial state, $|\psi_i\rangle = \sum_{k_i\ell_i} \psi^{k_i\ell_i}|\phi_{k_i}\rangle \otimes |\chi_{\ell_i}\rangle$, turns into the state

$$e^{-\frac{i}{\hbar}H_m t_m}|\psi_i\rangle = \sum_{kk_i\ell\ell_i} \psi^{k_i\ell_i} c^{k\ell}_{k_i\ell_i}|\phi_k\rangle \otimes |\chi_\ell\rangle. \tag{55}$$

This argument must be erroneous since it predicts the linear superposition of different states of the macroscopic display of the apparatus and leads to paradoxes as the Schrödinger's cat. The mistake we have committed is to treat a macroscopic collective degree of freedom as a microscopic one and we correct it by taking into account the environment.

B. Decoherence

Let us consider for the sake of simplicity a pure initial state of the apparatus and the environment, $|\chi_{k_i}\rangle \otimes |\eta_{\ell_i}\rangle$, after the measurement,

$$e^{-\frac{i}{\hbar}(H_A+H_e+H_{Ae}}|\chi_{\ell_i}\rangle \otimes |\eta_{m_i}\rangle = \sum_{\ell m} d^{\ell m}_{\ell_i m_i}|\chi_\ell\rangle \otimes |\eta_m\rangle. \tag{56}$$

To simplify the subsequent expressions we write this state in the Schmidt representation,

$$e^{-\frac{i}{\hbar}(H_A+H_e+H_{Ae}}|\chi_{\ell_i}\rangle \otimes |\eta_{m_i}\rangle = \sum_n d_n|\chi_n\rangle \otimes |\eta_n\rangle, \tag{57}$$

containing the pairwise orthonormal states, $\langle\chi_n|\chi_{n'}\rangle = \langle\eta_n|\eta_{n'}\rangle = \delta_{n,n'}$ which do not necessarily represent a complete basis. The relevant part of this state from the point of view of the observable, A, is the mixed state, defined by the reduced density matrix,

$$\rho_A = \sum_{nn'} d_n d^*_{n'} \langle\eta_{n'}|\eta_n\rangle |\chi_n\rangle\langle\chi_{n'}|, \tag{58}$$

c.f. appendix E, yielding the expectation value,

$$\mathrm{Tr}_A[A\rho_A] = \sum_{nn'} d_n d^*_{n'} \langle\eta_{n'}|\eta_n\rangle\langle\chi_{n'}|A|\chi_n\rangle. \tag{59}$$

The comparison of this expression with the expectation value, taken in the pure state, $|\chi\rangle = \sum_n d_n|\chi_n\rangle$,

$$\langle\chi|A|\chi\rangle = \sum_{nn'} d_n d^*_{n'} \langle\chi_{n'}|A|\chi_n\rangle, \tag{60}$$

indicates that the interference terms between the components $n \neq n'$ is suppressed in the mixed state by the relative environment state overlap, $\langle\eta_{n'}|\eta_n\rangle$.

To better understand eq. (60) consider the example of the measurement of the current, mentioned above, where the apparatus consists of the needle of the ammeter, $|\chi\rangle = |\theta\rangle$, θ being the angle of the needle. Let us take two different needle states, $|\theta_j\rangle$, $j = 1, 2$ with small $\Delta\theta = |\theta_1 - \theta_2|$, ignore the interaction between the air molecules and consider the air molecule components of the corresponding relative states, $|\eta_j\rangle$. The momentum of an air molecule changes by $\mathcal{O}(\Delta\theta)$ in scattering off the needle hence its overlap factor is $1 - c\Delta\theta + \mathcal{O}\left(\Delta\theta^2\right)$. The total overlap factor,

$$\langle\theta_1|\theta_2\rangle \approx (1 - c\Delta\theta)^N \approx e^{-cN\Delta\theta}, \tag{61}$$

$N \sim N_{Av} = 6 \cdot 10^{23}$ denoting the number of air molecules, decreases very fast with increasing $\delta\theta$. The strong suppression of the overlap with increasingly different needle states, $\langle\theta'|\theta\rangle \sim \delta(\theta - \theta')$, is called decoherence and is a necessary condition to avoid the linear superposition of macroscopically differing objects. The decoherence breaks up a coherent pure state into the set of pure states with no interference contributions among them,

$$|\psi\rangle\langle\psi| \to \sum_n p_n |\psi_n\rangle\langle\psi_n|, \tag{62}$$

since the reduced density matrix, being Hermitian, is diagonalizable, and the quantum mechanical expectation value, $\langle\psi_n|A|\psi_n\rangle$, appears in (59) with the classical probability weight, p_n. It is important to keep in mind that the decoherence, $\langle\eta_{n'}|\eta_n\rangle < 1$, results in non-unitary time evolution of the system which turns an initial pure system state into a mixed one.

Both decoherence and dissipation stem from the obsolete nature of the initial conditions, a loss of information, stored in the initial environment state. Both build up gradually and represent the transmutation of the environment time arrow to the observed system.

C. Choice

Rather than continuing to represent entangled states by the help of the Schmidt decomposition we return to our original basis, chosen in such a manner that $A|\chi_\ell\rangle = a_\ell|\chi_\ell\rangle$, and consider the reduced apparatus density matrix, corresponding to the state $|\Psi\rangle = \sum_{k\ell m} \Psi_{k\ell m}|\phi_k\rangle \otimes |\chi_\ell\rangle \otimes |\eta_m\rangle$ after the pre-measure and decoherence,

$$\rho_A = \sum_{k\ell\ell' m} \Psi_{k\ell m}\Psi^*_{k\ell' m}|\chi_\ell\rangle\langle\chi_{\ell'}|. \tag{63}$$

The environment induced decoherence, the summation over m, strongly suppresses the interference contributions between macroscopically different apparatus states. It is known that each measurement produces an element of the spectrum of the observable and what is left is to describe is this choice.

Instead of a detailed description we follow Neumann's idea and use the information that the eigenvalue a_ℓ was found by the measure to postulate that the density matrix of the apparatus after the complete measuring process is

$$\rho_\ell = \frac{P_\ell \rho P_\ell}{Tr_s[P_\ell \rho P \ell]} = P_\ell, \tag{64}$$

where $P_\ell = |\chi_\ell\rangle\langle\chi_\ell|$ is the projection operator to the ℓ-th eigenvector of A. It has been established experimentally that the choice violates special relativity thereby showing the non-local nature of quantum processes which we can not place within our usual deterministic world view. The choice is sometime called the collapse of the wave function because a non-trivial density matrix, (63), collapses onto a simple one, (64). It is clear that such a collapse leads to information loss and irreversibility hence it represents a statistical quantum time arrow.

The choice is the best kept secret of quantum mechanics and leads to sharp, so far unresolved contradictions between the ways we describe the microscopic and the macroscopic worlds. Let us mention, closing this topics, a possible resolution, namely the dominance of quantum physics. The measurement process can be viewed as a magnification of a microscopic event to a macroscopic one. We are used to imagine the latter as being governed by deterministic laws and predicting exact results for measurements, up to unavoidable and understandable error bars. The semiclassical solution of quantum field theories, combined with the renormalization group technique suggest

that the presence of a macroscopic number of degrees of freedom in the measuring process, N_{Av}, activates a variant of the Central Limit Theorem of probability theory and renders the relative second moment of an observable $\mathcal{O}\left(1/\sqrt{N_{Av}}\right)$. In other words, the extremely large value of the Avogadro number makes the quantum averages practically deterministic, following seemingly classical equations. According to this view the classical physics consists of the deterministic laws for the peak of such sharp probability distributions, reminiscent of thermodynamics. The special feature of the choice is that small changes of the the probability distribution, driven by the nonlinear effects of the apparatus, are magnified by the large number of degrees of freedom, cooperating in the measurement process which appears instantaneous because the very same large number generates unusually short time scales [1]. This is naturally a possible scenario only and the details remain to be worked out in details.

VI. COSMOLOGY

Cosmology is the widest framework to address the origin of the time arrow however we are satisfied here by mentioning few remarks owing to the complexity of the problem.

A. Initial conditions

It is not known whether gravity, the dynamical theory of the space-time, is subject of quantization. But the difference between the scenarios of quantum and classical gravity influences the very early Universe, up to few times the Planck's time, $6 \cdot 10^{-44}$sec only: The space-time of our Universe appeared through a quantum fluctuation or a singularity according to quantum and classical gravity, respectively. The continuation seems to be similar in both scenario, namely the Universe seems to be a cooling quantum gas of elementary particles in an expanding, classical space-time.

The contributions of gravity to the time arrow problem are the following:

- It describes the appearance of time as a cosmic book-keeping device.
- It justifies the use of the initial conditions.
- It generates horizons, surfaces which separate space-time regions with different causal structure and are semi-permeable for classical signals. The mechanism which prevents signals to traverse a horizon in certain direction follows from an elegant, smooth deformation of the causal structure, rather then from some singular energy barrier. The net result is a

time arrow, generated by the horizon, implying well defined initial conditions problems and distinctive thermodynamical and quantum mechanical effects.

B. Global time arrow

We have discussed several time arrows, electrodynamical, mechanical, thermodynamical and the quantum mechanical (decoherence and choice generated) which can be established in different regions of the space-time. Such a multiplicity of arrows raises the question of their consistency, the possibility of having a single, global time arrow within the causally connected regions of the space-time.

The initial condition problem, set by the early universe, generates a unique, global time arrow for phenomena, appearing on the cosmic scale. The electromagnetic time arrow is such a manifestations of the cosmic background radiation, extending to to our daily life. Another time arrow, generated by the initial conditions, is observed in mechanical systems. The thermodynamical time arrow follows from the ordered, low entropy initial state, thereby reducing the time arrow problem to the understanding of such an ordered feature of the initial state. The quantum mechanical time arrow points away in time from the environment auxiliary conditions and follows from the initial state, too.

Appendix A: Contour integrals

The brief recall of few theorems leading to the Fourier integral representation of translation invariant Green's functions is given below.

1. Cauchy-Riemann condition

The differentiability of a complex function, $f(z)$, the existence of the limit

$$f'(z) = \lim_{h\to 0} \frac{f(z+h) - f(z)}{h}. \tag{A1}$$

This seemingly simple definition implies much more than in real analysis because it assures that $f'(z)$ is independent of the phase of h. In other words, we find the same derivative as $|h| \to 0$, independently of the phase of h. The uniqueness of $f'(z)$ when $h = \eta$ and $h = i\eta$, $\eta \to 0$ being real,

$$\lim_{\eta\to 0} \frac{f(z+\eta) - f(z)}{\eta} = \lim_{\eta\to 0} \frac{f(z+i\eta) - f(z)}{i\eta}, \tag{A2}$$

assumes the form

$$\frac{\partial f_1}{\partial z_1} + i\frac{\partial f_2}{\partial z_1} = \frac{\partial f_2}{\partial z_2} - i\frac{\partial f_1}{\partial z_2} \tag{A3}$$

when the parametrization $f = f_1 + if_2$ and $z = z_1 + iz_2$ is used. The real and imaginary part of this equation,

$$\frac{\partial f_1}{\partial z_1} = \frac{\partial f_2}{\partial z_2}, \quad \frac{\partial f_2}{\partial z_1} = -\frac{\partial f_1}{\partial z_2}. \tag{A4}$$

yield the Cauchy-Riemann condition. A complex differentiable function is called holomorphic to distinguish complex differentiability from the simpler concept of the differentiability of real functions.

2. Cauchy's theorem

Let U be a simply connected open set of the complex plane (The openness is needed to move around in the vicinity of any point without leaving the region. A simply connected set is connected and any closed continuous loop, γ, can continuously be deformed to a point without leaving the domain. This property assures that there are no holes within U.) and $f(z)$ holomorphic on U. Cauchy's theorem states that the integral of $f(z)$ over γ in U is vanishing,

$$\oint_\gamma dz f(z) = 0. \tag{A5}$$

The complex line integral for a curve $\gamma : [0,1] \to \mathbb{C}$ is defined by

$$\int_\gamma dz f(z) = \int_0^1 ds \frac{d\gamma(s)}{ds} f(\gamma(s)). \tag{A6}$$

The proof starts by rewriting the loop integral,

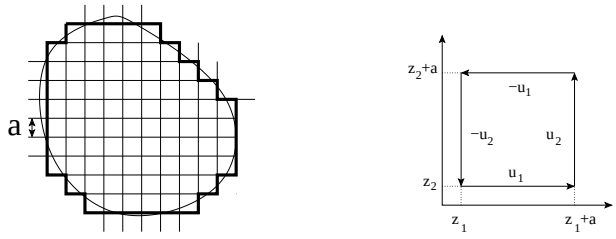
$$\begin{aligned} \oint_\gamma dz f(z) &= \oint (dz_1 + i dz_2)(f_1 + i f_2) \\ &= \oint_\gamma (dz_1 f_1 - dz_2 f_2) + i \oint (dz_1 f_2 + dz_2 f_1). \end{aligned} \tag{A7}$$

To evaluate the last line we apply Green's theorem,

$$\oint_\gamma d\boldsymbol{x}\boldsymbol{u} = \int_D d\boldsymbol{s}\boldsymbol{\nabla} \times \boldsymbol{u}, \tag{A8}$$

where the closed loop, γ, on the left hand side, is on the boundary of a simply connected region D, and is oriented in anticlockwise direction. The region, D, is chosen to be the $x_3 = 0$ plane, $\boldsymbol{x} = (z_1, z_2, 0)$ and the vector field, $\boldsymbol{u}(\boldsymbol{x}) = (u_1, u_2, 0)$, yields $\boldsymbol{\nabla} \times \boldsymbol{u} = (0, 0, \frac{\partial u_2}{\partial z_1} - \frac{\partial u_1}{\partial z_2})$ and

$$\oint_\gamma (dz_1 u_1 + dz_2 u_2) = \int_D dz_1 dz_2 \left(\frac{\partial u_2}{\partial z_1} - \frac{\partial u_1}{\partial z_2} \right). \tag{A9}$$



(a) (b)

FIG. 6: (a) The approximation of the integration contour γ by a piecewice linear function. (b) The enlarged view of an internal square.

To prove (A9) we approximate the closed loop γ by a rectangle made up by horizontal and vertical steps of size a as shown in Fig. 6 (a), the limit $a \to 0$ will be performed at the end. The left hand side is a times the sum of u_1 (u_2) long the horizontal (vertical) steps along the approximate boundary. The right hand side is the sum of the surface integral, calulated for each square within the approximate boundary. The integral for a given square,

$$\int_{z_1^-}^{z_1^+} dz_1 \int_{z_2^-}^{z_2^+} dz_2 \left(\frac{\partial u_2}{\partial z_1} - \frac{\partial u_1}{\partial z_2} \right) = \int_{z_2^-}^{z_2^+} dz_2 [u_2(z_1^+, z_2) - u_2(z_1^-, z_2)] - \int_{z_1^-}^{z_1^+} dz_1 [u_1(z_1, z_2^+) - u_1(z_1, z_2^-)], \quad \text{(A10)}$$

written in the form

$$\int_{z_1^-}^{z_1^+} dz_1 \int_{z_2^-}^{z_2^+} dz_2 \left(\frac{\partial u_2}{\partial z_1} - \frac{\partial u_1}{\partial z_2} \right) = a[u_1(z_1^-, z_2^-) + u_2(z_1^+, z_2^-) - u_1(z_1^-, z_2^+) - u_2(z_1^-, z_2^-)] + \mathcal{O}\left(a^2\right), \quad \text{(A11)}$$

shows that the right hand side can be approximated by summing this elementary sum over the internal squares. Since each internal line is shared by two internal squares where the contibution of thisline emerges with opposite signe such a sum is reduces to the sum of the lines along the perimeter. This argument assumes that there are no holes within the regions encircled by γ since their perimeter contribution would remain uncancelled.

The application of (A9) to the real (imaginary) part with $u_1 = f_1$, $u_2 = -f_2$ ($u_1 = f_2$, $u_2 = f_1$) of (A7) yields

$$\oint_\gamma dz f(z) \;=\; -\int_D dz_1 dz_2 \left(\frac{\partial f_2}{\partial z_1} + \frac{\partial f_1}{\partial z_2} \right) + i \int_D dz_1 dz_2 \left(\frac{\partial f_1}{\partial z_1} - \frac{\partial f_2}{\partial z_2} \right) = 0 \quad \text{(A12)}$$

and the vanishing follows from the Cauchy-Riemann equations.

The main use of Cauchy's theorem is that a complex integral,

$$I_\gamma = \int_\gamma dz f(z), \quad \text{(A13)}$$

remains unchanged when the contour of integration, γ, is deformed without crossing singularities. To prove this statement first note that we have $I_{\gamma^{-1}} = -I_\gamma$ where γ^{-1} denotes the contour γ, followed in the oppposite direction, i.e. $\gamma^{-1}(s) = \gamma(1-s)$ where $0 \le s \le 1$ is a parameter of the curve $\gamma : [0,1] \to \mathbb{C}$. Let us now suppose that the curve γ' can be obtained by deforming γ without traversing singularities and keeping the end points unchanged. The curve, obtained

by following γ and γ'^{-1} is closed and encircles a simply connected holomoprhic domain hence $I_\gamma + I_{\gamma'^{-1}} = I_\gamma - I_{\gamma'} = 0$.

Cauchy's theorem can be used to show that if a function is holomorphic within an open and simply connected domain D then it is infinitely many time differentiable and analytic, i.e. can be represented by an absolutely and uniformly convergent power series

$$f(z) = \lim_{N\to\infty} \sum_{n=0}^{N} f_n (z - z_0)^n \tag{A14}$$

within the convergence radius of the series, $z, z_0 \in D$, $|z - z_0| < r$ (this latter is important because it allows us to exchange the order of the limit and the integration and differentiation of $f(z)$). The argument is based on the relation

$$f(z) = \frac{1}{2\pi i} \oint_\gamma du \frac{f(u)}{u - z}, \tag{A15}$$

where $z \in D$ and γ is a circle of infinitesimal radius, centered at z. Cauchy's theorem allows us to increase the circle to a finite radius as long as γ stays within D. It is easy to check that the integrand converges absolutely and uniformly for z within γ hence we can calculate the subsequent derivatives, $d^n f(z)/dz^n$ by derivating the integrand.

3. Residuum theorem

The residue of a function $f(z)$ at z_0 is $Resf(z_0) = \lim_{z\to z_0}(z - z_0)f(z)$ if the limit exist. The residue is vanishing for holomorphic function but can be non-vanishing at some singularity. Let us assume that $f(z)$ is holomorphic on a a simply connected domain, D, except at a finite set of discrete points, $\{z_1, \ldots, z_N\}$. The residue theorem states that the loop integral over a loop within D, calculated in anticlockwise direction is the sum of the residues of the function times $2\pi i$,

$$\oint_\gamma dz f(z) = 2\pi i \sum_{n=1}^{N} \nu_\gamma(z_n) Resf(z_n), \tag{A16}$$

where $\nu_\gamma(z)$ denotes the winding number,

$$\nu(z) = \frac{1}{2\pi i} \oint_\gamma dz' \frac{1}{z' - z}, \tag{A17}$$

the number of times γ travels counterclockwise around z. To understand this definition better let us consider a closed loop, γ, around z, $z' - z = r(\alpha)e^{i\phi(\alpha)}$, parameterized by the angle $0 \le \alpha \le 2\pi$,

$$\begin{aligned} \nu(z) &= \frac{1}{2\pi i} \int_0^{2\pi} d\alpha \frac{(\frac{dr}{d\alpha} + ir\frac{d\phi}{d\alpha})e^{i\phi}}{re^{i\phi}} \\ &= \frac{1}{2\pi i} \int_0^{2\pi} d\alpha \frac{d\ln r}{d\alpha} + \frac{1}{2\pi} \int_0^{2\pi} d\alpha \frac{d\phi}{d\alpha}. \end{aligned} \tag{A18}$$

The fundamental difference between the variables r and ϕ is that the former is an arbitrary non-negativ number, $r(0) = r(2\pi)$, and latter is defined in the interval $[-\pi, \pi]$ and is periodic, $\phi(2\pi) =$

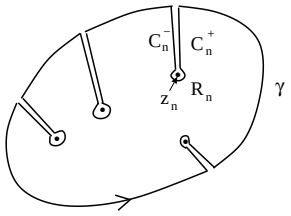


FIG. 7: The deformation of a closed integration contour by excluding the singularities.

$r(0) + 2\pi\nu$. The winding number, ν, defined in such a manner is a topological quantity, i.e. it remains invariant under the continuous deformation of the loop, γ. Since $\nu_\gamma(z) = 0$ outside of γ the summation in the residue theorem is over the singularities encircled by the loop only.

The proof of eq. (A16) consists of applying Cauchy's theorem for the contour γ', constructed by excluding the singular points from the domain of integration as shown on Fig. 7: The integrals over the slightly displaced parallel lines cancel and the integral around each pole gives the corresponding residuum contribution.

Appendix B: Green's functions

The Green's functions provide a clear and compact solution of linear differential equations. Let us start with an inhomogeneous real linear differential equation, $L(\partial_t)x = j$, for $x(t)$. The Green's function of this equation is defined by

$$L(\partial_t)G(t,t') = \delta(t-t'). \tag{B1}$$

The generalized function, the Dirac-delta, is defined by the equation

$$f(t) = \int dt' \delta(t-t') f(t'), \tag{B2}$$

holding for infinitely many differentiable test functions $f(t)$ with compact support. The multiplication of eq. (B1) by $j(t')$ and the integration over t' yields $L(\partial_t)x = j$ for

$$x(t) = \int dt' G(t,t') j(t'). \tag{B3}$$

This is only a formal solution because it is ill-defined on the the null space of the operator L, consisting of the eigenfunctions with vanishing eigenvalue, $L(\partial_t)\phi(t) = 0$. In fact, the Dirac-delta can be interpeted as the unit operator, $f = \mathbb{1}f$, in the space of test functions according to (B2) hence $G = L^{-1}$ and the inverse is not defined in the null space.

The ill-defined null-space dynamics leads to the following difficulties in the physical applications where the differential equation is our linear equation of motion:

- The null-space consists of the solution of the equation of motion without external source, it contains the physically most important trajectories.
- The action,
$$S[x] = \int dt \left[\frac{1}{2} x(t) L(\partial_t) x(t) - x(t) j(t) \right], \tag{B4}$$
reproduces our differential equation as an Euler-Lagrange equation. L can be written as the sum of symmetric and antisymmetric parts, $L = L^s + L^a$, $L^{\overset{s}{a}} = (L \pm L^{\mathrm{tr}})/2$, and the antisymmetric part does not contribute to the action. The remaining symmetric part, $G^{-1s}(t-t') = G^{-1s}(t'-t)$, yields symmetric Green's function, $G^s(t-t') = G^s(t'-t)$, violating causality. In fact, an external force, $j(t) = j_0 \delta(t-t_0)$, produces effects both for $t < t_0$ and $t > t_0$ according to the solution (B3).
- We can write the solution of the equation of motion in the form of a spectral integral,
$$x(t) = \int d\lambda x_\lambda \phi_\lambda(t), \tag{B5}$$
where $L\phi_\lambda = \lambda\phi$ and L is assumed to be a Hermitian operator whose eigenvectors yield a basis. The source admits a similar linear decomposition, yielding the equation of motion, $\lambda x_\lambda = j_\lambda$, which in turn shows that the restoring force, j_λ/λ, acting on the null space mode with $\lambda = 0$ is singular and a regular solution can be found for the particular kind of external force, $j_0 = 0$. A source with $j_0 \neq 0$ which produces resonance leads to ill-defined solution.

The problem can be avoided by using the auxiliary, i.e. initial and/or final conditions and Green's function to fix $x(t)$ within and beyond the null space, respectively. For this end we use the usual decomposition, $x(t) = x_h(t) + x_{ih}(t)$, where $x_h(t)$ ($x_{ih}(t)$) denotes a solution of the homogeneous (inhomogeneous) equation. Hence we need a Green's functions which produces $x_{ih}(t)$ with vanishing auxiliary conditions. The usual way to make these Green's functions well defined one removes the null space of the equation of motion by the modification $L \to L_\epsilon = L + i\epsilon$ and the limit $\epsilon \to 0$ is performed at the end of the calculation. This step introduces an $\mathcal{O}(\epsilon)$ error in the equation of motion, an acceptable violation since ϵ is removed at the end. However such a regularization of Green's function leaves a finite trace behind, the breakdown of the invariance under time reversal and the emergence of retarded and advanced solutions.

1. Harmonic oscillator

We start with the simplest case, a harmonic oscillator, defined by the equation of motion,

$$m\ddot{x}(t) = -m\omega_0^2 x(t) - j(t), \tag{B6}$$

where the external force, j, is introduced to diagnose the system.

The Fourier transformation, an essential tool in solving linear differential equations, can be facilitated by using the Fourier representation of the Dirac-delta,

$$\delta(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-ikx}. \tag{B7}$$

In fact, the insertion of the identity, expressed by this form of the Dirac-delta,

$$\begin{aligned} f(t) &= \mathbb{1}f(t) = \int \frac{d\omega}{2\pi} dt' e^{-i\omega(t-t')} f(t') = \int \frac{d\omega}{2\pi} e^{-i\omega t} \tilde{f}(\omega), \quad \tilde{f}(\omega) = \int dt e^{i\omega t} f(t) \\ \tilde{f}(\omega) &= \mathbb{1}\tilde{f}(\omega) = \int \frac{d\omega}{2\pi} dt' e^{-i\omega(t-t')} f(t') = \int \frac{d\omega}{2\pi} e^{i\omega t} f(t), \quad f(t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} \tilde{f}(\omega) \end{aligned} \tag{B8}$$

shows the equivalence of (B2) and Fourier's theorem.

The solution (B3) can be written for

$$x(\omega) = \int dt e^{-i\omega t} x(t), \tag{B9}$$

as

$$x(\omega) = \tilde{D}(\omega) j(\omega) \tag{B10}$$

where $\tilde{D}(\omega) = \frac{1}{m(\omega^2 - \omega_0^2)}$ denotes the Green's function. Such a result is not uniquely defined because the denominator is vanishing within the null space of the equation of motion, $\omega = \pm\Omega$. The null space dynamics is fixed by the auxiliary conditions, given either as initial or final conditions, $x(-\infty) = \dot{x}(-\infty) = 0$ or $x(\infty) = \dot{x}(\infty) = 0$, respectively. Non-trivial auxiliary conditions can be satisfied by adding appropriate terms to the external force, $j(t)$. The initial condition problem is solved by the help of the retarded Green's function, $D^r(t) \sim \Theta(t)$, containing a null space modes which cancel the initial coordinate and velocity.

The calculation of the Green's function of a harmonic oscillator is a nice application of the residue theorem. The poles of $\tilde{D}(\omega)$, $\omega_\pm = \pm\omega_0$, can be shifted infinitesimally off from the real axis in different directions, $\omega_\pm \to \omega_\pm = \pm\omega_0 + \sigma i\epsilon$, where $\sigma = \pm 1$ and $\epsilon = 0^+$, yielding four different Green's functions,

$$D_{\sigma\sigma'}(t) = \lim_{\Omega\to\infty} \int_{-\Omega}^{\Omega} \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{m[(\omega - \omega_0 - i\sigma\epsilon)(\omega + \omega_0 - i\sigma'\epsilon)}. \tag{B11}$$

We may close the integration contour over either the upper or the lower half circle as shown in Fig. 8. We want the integral over the real axes only therefore the semicircle contribution should vanish as $\Omega \to \infty$. It is easy to see that this is the case for upper or the lower semicircle for $t < 0$ and $t > 0$, respectively. This rule determines the contour and yields

$$\begin{aligned} D_{++}(t) &= i\Theta(-t)\frac{e^{-i\omega_0 t} - e^{i\omega_0 t}}{2m\omega_0} e^{\epsilon t} = \Theta(-t)\frac{\sin\omega_0 t}{m\omega_0} e^{\epsilon t} = D^a(t) \\ D_{+-}(t) &= i\frac{\Theta(t)e^{i\omega_0 t} + \Theta(-t)e^{-i\omega_0 t}}{2m\omega_0} e^{-\epsilon|t|} = i\frac{e^{i\omega_0|t|}}{2m\omega_0} e^{-\epsilon|t|} = D_F^*(t) \\ D_{-+}(t) &= -i\frac{\Theta(t)e^{-i\omega_0 t} + \Theta(-t)e^{i\omega_0 t}}{2m\omega_0} e^{-\epsilon t} = -i\frac{e^{-i\omega_0|t|}}{2m\omega_0} e^{-\epsilon|t|} = D_F(t) \\ D_{--}(t) &= -i\Theta(t)\frac{e^{-i\omega_0 t} - e^{i\omega_0 t}}{2m\omega_0} e^{-\epsilon t} = -\Theta(t)\frac{\sin\omega_0 t}{m\omega_0} e^{-\epsilon t} = D^r(t), \end{aligned} \tag{B12}$$

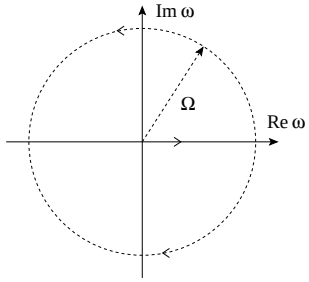


FIG. 8: Two different ways to close the integration contour on the complex frequency plane.

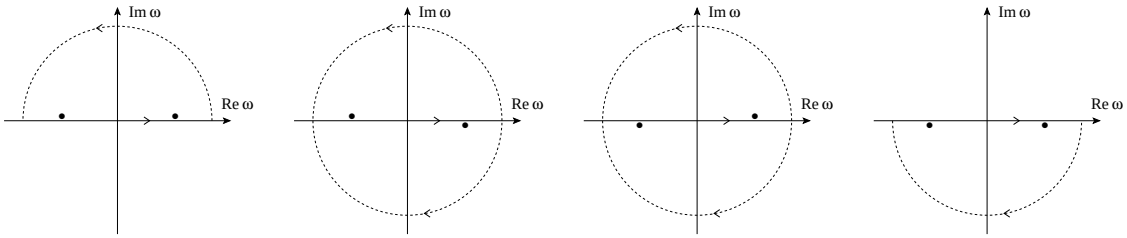


FIG. 9: The poles of the four kinds of Green's function of eqs. (B12).

defining the advanced (D^a), the Feynman (D_F) and the retarded (D^a) Green's functions. The retarded and advanced Green's functions are used to construct the solution of initial and final state problems and the D_F gives the solution of the mixed auxiliary condition, with vanishing initial and final coordinates and is used only in quantum mechanics.

2. Electromagnetic field

The formal Green's function of the wave equation (8),

$$D(x-x') = \int \frac{d^4q}{(2\pi)^4} e^{-iq(x-x')} \tilde{D}(q), \tag{B13}$$

is given by

$$\tilde{D}(q) = \begin{cases} -\frac{1}{q^2} & q^2 \neq 0, \\ ? & q^2 = 0, \end{cases} \tag{B14}$$

$q^2 = q^{02} - \boldsymbol{q}^2$. The retarded Green-function, $D^r(x,y) \approx \Theta(x^0 - y^0)$, is found by shifting the poles of $\tilde{D}(q)$ below the real frequency axis,

$$\begin{aligned}
D^r(x) &= -\int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{kx}} \int \frac{dk_0}{2\pi} \frac{e^{-ick_0t}}{(k_0 + i\epsilon - |\boldsymbol{k}|)(k_0 + i\epsilon + |\boldsymbol{k}|)} \\
&= i\Theta(t) \int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{kx}} \left(\frac{e^{-ickt}}{2k} - \frac{e^{ickt}}{2k} \right) \\
&= \frac{i\Theta(t)}{(2\pi)^3} \int dk k^2 d\phi d(\cos\theta) e^{ikr\cos\theta} \frac{e^{-ickt} - e^{ickt}}{2k} \\
&= \frac{i\Theta(t)}{(2\pi)^2} \int dk k^2 \frac{e^{ikr} - e^{-ikr}}{ikr} \frac{e^{-ickt} - e^{ickt}}{2k} \\
&= \frac{\Theta(t)}{2(2\pi)^2 r} \int_0^\infty dk (e^{ikr} - e^{-ikr})(e^{-ickt} - e^{ickt}) \\
&= \frac{\Theta(t)}{8\pi r} \int_{-\infty}^{\infty} \frac{dk}{2\pi} (e^{ik(r-ct)} + e^{ik(-r+ct)} - e^{-ik(r+ct)} - e^{ik(r+ct)}) \\
&= \frac{\Theta(t)}{4\pi r} [\delta(-r + ct) - \delta(r + ct)] \\
&= \frac{\delta(ct - r)}{4\pi r}.
\end{aligned} \tag{B15}$$

The advanced Green's function is given by

$$\begin{aligned}
D^a(x) &= -\int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{kx}} \int \frac{dk_0}{2\pi} \frac{e^{-ick_0t}}{(k_0 - i\epsilon - |\boldsymbol{k}|)(k_0 - i\epsilon + |\boldsymbol{k}|)} \\
&= i\Theta(-t) \int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{kx}} \left(\frac{e^{ickt}}{2k} - \frac{e^{-ickt}}{2k} \right) \\
&= \Theta(-t) \frac{\delta(r + ct) - \delta(-r + ct)}{4\pi r} \\
&= \frac{\delta(ct + r)}{4\pi r}.
\end{aligned} \tag{B16}$$

Finally the relativistically invariant form of both Green's functions is

$$\begin{aligned}
\overset{r}{D^a}(x) &= \Theta(\pm t) \frac{\delta(ct \mp r)}{4\pi r} \\
&= \Theta(\pm t) \frac{\delta(ct + r) + \delta(ct - r)}{4\pi r} \\
&= \Theta(\pm t) \frac{\delta(c^2t^2 - r^2)}{2\pi} \\
&= \Theta(\pm x^0) \frac{\delta(x^2)}{2\pi}.
\end{aligned} \tag{B17}$$

Since $D^a(x,y) = D^{\mathrm{rtr}}(x,y) = D^r(y,x)$ the symmetric and antisymmetric parts of the Green's functions

$$\overset{n}{D^f} = \frac{1}{2}(D^r \pm D^a) \tag{B18}$$

give the solutions of the inhomogeneous and homogeneous equation, respectively. The inhomogeneous Green-functions are connected by the relation

$$\overset{r}{D^a}(x,y) = 2D^n(x,y)\Theta(\pm(x^0-y^0)) \tag{B19}$$

where the near field Green's function is

$$D^n(x) = \frac{\delta(x^2)}{4\pi} \tag{B20}$$

according to Eq. (B17). The Fourier representation of the homogeneous far Green's function can be obtained by considering the difference of the second lines in Eqs. (B15) and (B16),

$$\begin{aligned} D^f(x) &= \frac{1}{4\pi}\delta(x^2)\epsilon(x^0) \\ &= -\frac{i}{2}\int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{kx}}\left(\frac{e^{ickt}}{2k} - \frac{e^{-ickt}}{2k}\right) \\ &= \frac{i}{2}\int \frac{d^4k}{(2\pi)^3} e^{-ikx}\frac{\delta(k_0-|\boldsymbol{k}|)-\delta(k_0+|\boldsymbol{k}|)}{2|\boldsymbol{k}|} \\ &= \frac{i}{2}\int \frac{d^4k}{(2\pi)^3} e^{ikx}\delta(k^2)\epsilon(k_0) \end{aligned} \tag{B21}$$

where $\epsilon(x) = \text{sign(x)}$. A useful relation satisfied by this Green-function is

$$\begin{aligned} \partial_{x^0} D^f(x)_{x^0=0} &= \frac{1}{2}\int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{kx}} k_0 \frac{\delta(k_0-|\boldsymbol{k}|)-\delta(k_0+|\boldsymbol{k}|)}{2|\boldsymbol{k}|} \\ &= \frac{1}{2}\int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{kx}} \frac{1}{2}[\delta(k_0-|\boldsymbol{k}|)+\delta(k_0+|\boldsymbol{k}|)] \\ &= \frac{1}{2}\delta(\boldsymbol{x}) \end{aligned} \tag{B22}$$

The difference between the retarded and the advanced Green's function, the sign of the imaginary part of the denominator of the frequency integral, leads to different sign of the null space contributions, $\delta(q^2)$, to the Fourier integral. This observation indicates that the regularization of the divergent integrand, the treatment of the null space modes and the implementation of the auxiliary conditions, indeed correspond to the same problem.

Appendix C: Liouville's theorem

Let us consider a classical system, described by the canonical variables, $(\boldsymbol{q},\boldsymbol{p})$, and the Hamiltonian, $H(\boldsymbol{p},\boldsymbol{q})$. The Hamilton equations,

$$\dot{\boldsymbol{q}} = \frac{\partial H(\boldsymbol{p},\boldsymbol{q})}{\partial \boldsymbol{p}}, \quad \dot{\boldsymbol{p}} = -\frac{\partial H(\boldsymbol{p},\boldsymbol{q})}{\partial \boldsymbol{q}}, \tag{C1}$$

generate the flow, $(\boldsymbol{q}(t_i), \boldsymbol{p}(t_i)) \to (\boldsymbol{q}(t), \boldsymbol{p}(t))$, in the phase space.

Liouville's theorem states that this flow preserves the volume in the phase space. The proof starts with a lemma about volume dependence, generated by the solution of the equation of motion, $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})$. We introduce

$$\Gamma(R) = \int_R dx, \tag{C2}$$

the volume of the region R and show that

$$\frac{d\Gamma(R(t))}{dt} = \int_{R(t)} dx \boldsymbol{\nabla} \boldsymbol{f}(\boldsymbol{x}(t)). \tag{C3}$$

The volume at time t is given by

$$\Gamma(R(t)) = \int_{R(t_i)} dx \det \frac{\partial \boldsymbol{x}(t)}{\partial \boldsymbol{x}(t_i)} \tag{C4}$$

and the approximate solution, $\boldsymbol{x}(t + \delta t) \approx \boldsymbol{x}(t) + \delta t \boldsymbol{f}(\boldsymbol{x}(t))$, yields

$$\frac{\partial \boldsymbol{x}(t + \delta t)}{\partial \boldsymbol{x}(t)} \approx \mathbb{1} + \delta t \frac{\partial \boldsymbol{f}(\boldsymbol{x}(t))}{\partial \boldsymbol{x}(t)} \tag{C5}$$

The $\mathcal{O}(\delta t)$ part of this matrix is the sum of the $\mathcal{O}(\delta t)$ diagonal elements on the right hand side, giving

$$\det \frac{\partial \boldsymbol{x}(t + \delta t)}{\partial \boldsymbol{x}(t)} \approx 1 + \delta t \boldsymbol{\nabla} \boldsymbol{f}(\boldsymbol{x}(t)). \tag{C6}$$

The volume after infinitesimal time evolution,

$$\Gamma(R(t + \delta t)) = \int_{R(t)} dx [1 + \delta t \boldsymbol{\nabla} \boldsymbol{f}(\boldsymbol{x}(t))] \tag{C7}$$

gives the derivative (C3).

Liouville's theorem, $\dot{\Gamma}(R) = 0$, now follows by applying this lemma in the phase space to the flow of Hamilton's equations because the second derivative of the Hamiltonian is a symmetric matrix.

Appendix D: Probability and Information in Physics

The use and the interpretation of the probability in physics is not as simple as one would have imagined. Furthermore the relevance of of information in physics has been recognized gradually only. These two concepts are surveyed briefly below.

1. Traditional and Bayesian probabilities

The probability theory, a chapter of mathematics, starts with a set of elementary events, E, and construct its subsets as combined events. The total event space, L, form a σ-algebra, namely it is closed under forming the complement, $A \in L \Rightarrow A^c \in L$ where $A \cup A^c = E$, and the union of countable many subsets, $A_i \in L \Rightarrow \cup_i A_i \in L$. The probability is a measure, an assignment of a number, to each events, and satisfies three axioms: (i) The probabilities are real, non-negative, finite numbers. (ii) At least one event is assumed to be realized, that receives the probability value 1. (iii) The the probability is additive for mutually exclusive events. (iv) An event or its complement is always realized, $p(A) + p(A^c) = 1$. This set of conditions lead to Kolmogorov's theory of probability.

Note that this definition is about the use of probability without providing a constructive definition and leaves possible different interpretations of the actual probability values. The mathematical statics is based on the definition of the probability, given by the law of large numbers, This law states that the empirical rate of the realization of an event approaches the probability in the limit of infinitely many independent trials. This definition is consistent with the subsequent use of the probability however remains circular because it is stated in probabilistic manner by showing that the probability of a fixed deviation between the empirical rate and the probability tends to zero. Such a view of the probability leads to the construction of random variables, which assume values with an empirical rate, given by the law of large numbers. The Bayesian view is that the probability is a measure of our partial knowledge. This is supported by Bayes' theorem,

$$p(A|B) = \frac{p(B|A)p(A)}{p(B)}, \tag{D1}$$

a trivial result of the definition

$$p(A|B) = \frac{p(B \cap A)}{p(B)}, \tag{D2}$$

of the conditional probability of A, assuming B. The Bayesian interpretation of eq. (D1) is that our state of knowledge, encoded by the probability distribution $p(A)$, changes to $p(A|B)$ is we are sure of B. No random variables are needed for this interpretation.

The only discipline in Natural Sciences which claims a constructive definition of the probability is Quantum Mechanics, in particular Born's rule. There are three reasons to interpret that probability in the Bayesian manner. The first two consist of pointing out an undesired features of the probability, defined by the law of large numbers in the classical and the quantum domains.

(i) Let us suppose that the probability of an event is defined by the repeated observation of the event in a series of independent trials. Is this probability an objectively existing property as say the mass or the coordinate of a particle in classical physics? According to the classical laws of physics the latter properties are known with a certain error bars after the measurement. However the determination of the probability by the law of large numbers requires infinitely many trials and the measurement, carried out in a finite time lapse, leaves an inestimable error.

(ii) An important condition of the law of large number, namely the independence of the trials, can not be guaranteed in the quantum case. In fact, the production of a set of independent, equivalently prepared systems is highly irrealistic due to the unavoidable entanglement, emerging between the preparing device and the observed systems. Such an entanglement correlates the observed systems, too. If there are doubts about the ensemble interpretation of the probability, given by Born's rule, then one is left with the assumption that the probability corresponds to a single observation. However then intriguing, open question remains about the physical interpretation of the probability of a single, non-repeatable event.

(iii) The third argument is to point out the absence of random variables in quantum domain. Consider for instance the spin operators of a particle of spin $S = 3/2$, satisfying the relation

$$\frac{15}{4}\hbar^2 \mathbb{1} = S_x^2 + S_y^2 + S_z^2 \tag{D3}$$

for the spin operators, $\boldsymbol{S}$, with spectrum $\pm\hbar/2, \pm 3\hbar/2$. One can not choose eigenvalues for all the three spin operators which satisfies eq. (D3). This complication, a well known result of Heisenberg's uncertainty principle for the operators $[S_a, S_b] = \hbar \sum_c \epsilon_{abc} S_c$, indicates that the proper interpretation of the uncertainty principle is the impossibility of having full, exhausting knowledge in the quantum world.

2. Classical and quantum probabilities

We have arrived at an important difference of the quantum and the classical probabilities: Both are related to missing information however that information exists in the deterministic classical world "out there" and is nonexistent in the quantum case. The probability arises in classical physics due to some limitation of the observer and in Quantum Mechanics due to the specific structure or reality which always remains inaccessible, ill defined for macroscopic measuring devices.

An interesting, related formal difference of the classical and quantum probabilities is the space of events. On the one hand, this space is a σ-algebra for the classical probabilities, satisfying

Kolmogorov's axioms, whose structure reflects the properties of set theories which in turn is based on the existence of stable properties, a characteristic of macroscopic, classical physics. On the other hand, the properties of a microscopic system are defined by linear subspaces in Quantum Mechanics. There is a difference of the axioms, satisfied by subsets and by linear subspaces, namely the distributivity is missing in the latter case. In other words, the quantum probabilities correspond to a non-distributive event set.

Such a double layered structure of the probability emerges in the density matrix where the quantum fluctuations arise from the pure states and the classical uncertainty is encoded by the probability of finding the system in a given pure state.

3. Probability as the extension of logic

In the absence of any uncertainty we use our knowledge to generate new statements and the laws of this process, called deductive inference, is the subject of mathematical formal logic. The founders of probability theory, James Bernoulli. Thomas Bayes and Pierre Simon Laplace looked upon probability as the generalization of this scheme in case of some uncertainty. However the latter could not prove that such a use of probability needs the assumptions, given at the beginning of section D 1 and Bayes' law. Such a missing link was found by David Cox and presented in physical context by Edwin Jaynes in the XX.-th century. In the meantime the mathematical model, realizing the probabilities, arising from the axioms of section D 1, was created by the help of random variables and formalized by Kolmogorv's theory.

In view of the remarks of the previous section about the preference of the Bayesian view of the probability in physical sciences we employ that that interpretation to the inference problem. The deductive inference, called Boolean logic, can be regarded as a result of the simplest, $p \in \{0, 1\}$ probability assignment. The 0 and 1 valued probability distributions contain no uncertainty. In the daily life we maneuver with partial information and make statements with uncertainties. The laws of this process, called plausible inference, is provided by the Bayesian probability theory. The set of events is now replaced by the set of statements ($\cup \to \vee$: "or", $\cap \to \wedge$: "and" and $A^c \to \bar{A}$: "negation of A") which is a σ-algebra for the classical probability.

The usual application of the Bayesian probability theory consists of the following two related problems: 1. Inference: How to assign the probability values of statements when we have a certain knowledge? 2. Update: How to change the probabilities if our knowledge enhanced? The first problem, phrased in physical terms, is the identification of the state of our system upon

of our knowledge. It relies on σ-algebra based statements in classical Statistical physics. There are indications that the most satisfactory interpretation of the formalism of Quantum Mechanics is to consider it as a systematic and optimized treatment of probabilities, arising from a non-distributive statement structure. A more detailed discussion of the classical case, the Maximal Entropy Principle, is presented in section D 5.

We turn now the simpler problem 2, a simple model of the learning process. For that end we assume that we posses the knowledge I at the initial state which has enabled us to form the probability distribution, $p(H_i|I)$, for a set of exclusive and exhaustive hypotheses, H_i, $\sum_i p(H_i|I) = 1$. We acquire new knowledge in the form of some data, D, and find the updated probability by the help of Bayes' theorem,

$$p(H_i|D \wedge I) = \frac{p(D|H_i \wedge I)p(H_i|I)}{p(D|I)}, \tag{D4}$$

where $p(H_i|I)$ denotes the prior probability, used before the new data, $p(D|H_i \wedge I)$ is called the likelihood function of the hypothesis H_i and the result, $p(H_i|D \wedge I)$ is the posterior probability. As a simple application of this result we consider the hypothesis testing, the determination of the best fitting hypothesis to the new data. The ratio of the probability of two hypotheses,

$$\frac{p(H_1|D \wedge I)}{p(H_2|D \wedge I)} = \frac{p(D|H_1 \wedge I)}{p(D|H_2 \wedge I)} \cdot \frac{p(H_1|I)}{p(H_2|I)}, \tag{D5}$$

contains the ratio of the likelihoods and the priors. There are two simple extremities: If the initial information does no single out any hypothesis then the second factor is unity and the best fitting hypothesis belongs the maximum likelihood. If the data seems unrelated to the hypotheses then the first factor is unity and the sought hypothesis is determined by the initial knowledge.

4. Information

To turn the foregoing qualitative discussion into a quantitative algorithm of determining the probability assignment of a given knowledge one needs a quantitative measure of information, represented by some knowledge. The first, mathematically well defined use of information is due Claude Shannon, an electric engineer, who sought a characterization of the usefulness of data compression and presented his proposition in his paper, entitled "A Mathematical Theory of Communication", in 1948. John Neumann has pointed out immediately that Shannon's measure of information is equivalent with the entropy, used in physics. The Maxwell demon paradigm, revisited by Leo Szilárd in 1929, actually has given indications that the information plays an important role in

statistical physics and an information based foundation of equilibrium statistical physics has been worked out by Edwin Jaynes in 1957.

First of all one has to clarify the meaning of the word, "information". How to find a role for a concept of human communication in natural science which is supposed to be objective, i.e. independent of the observer? The answer comes from a more careful view of the role, the humans play in this issue. They receive certain information, use their intelligence and react accordingly. We can assign machines to function in a similar manner. An important lesson, to be remembered in the critical discussion of Maxwell's demon, is that both the human being and the machine obey the physical laws. After having eliminated the role, played by the intelligence, we can turn to the meaning of the information. Information denotes data acquisition, transfer, storage and finally use by mathematically well defined algorithms. Loosely speaking information stands for data and the rules of their use.

Since the probability appears due to he missing information it is natural to seek a quantitative measure of the latter, I, in terms of the probability distribution of the elementary events. We present this construction in the case of classical probability by considering a series of independent trials whose outcome, $j \in [1, \ldots, n]$, follows the probability distribution $p = (p_1, \ldots, p_n)$. We use discrete random variables here for the sake of simplicity. To be more specific, let us consider the case of a ball which can be placed in one of n equivalent urns. Once the ball is hidden in one of the urns, in each if them with the same probability $p_j = 1/n$, our missing information, I_n, can be obtained by requiring the following properties:

1. $I_{n'} > I_n$ for $n' > n$

2. $I_1 = 0$

3. Composition law: Let us place in each of the n urns m smaller urns. The place of a ball is specified by the doublet (j, k), $j = 1, \ldots, n$, $k = 1, \ldots, m$ and we miss information about both j and k,

$$I_{nm} = I_n + I_m. \tag{D6}$$

The simple solution,

$$I = \ln \Omega, \tag{D7}$$

is unique up to a multiplicative constant among the continuous functions where the "phase space", $\Omega = n$, denotes the number of accessible states.

In the case of a non-constant probability distributions we follow a heuristic argument to generalize the composition law, mentioned as point 3 above. We start again by placing a ball with equal probability into one of N urns. However we regroup the urns into n groups, ℓ_j denoting the number of urns in the j-th group, $\sum_j \ell_j = N$. The ball is then found in the group j with probability $p_j = \ell_j/N$. We now seek the missing information $I[p]$ about the position of the ball with respect to the groups only. The total information missing is $I_t = \ln N$ and we have to remove from it the information I_g which is missing due to the different possible positions within the groups. The average of the information, to be removed is

$$\langle I_g \rangle = \sum_{j=1}^{n} p_j \ln \ell_j \tag{D8}$$

according to Eq. (D7), leading to

$$I[p] = I_t - \langle I_g \rangle = -\sum_{j=1}^{\ell} p_j \ln p_j. \tag{D9}$$

Another, perhaps more illuminating argument is to consider the series of N symbols, $j_1, \ldots, j_N$, chosen from a fixed set of n object, say $j_k \in \{1, \ldots, n\}$, in such a manner that $P(j_k = j) = p_j$. What is the missing information about a series, subject of a given probability distribution? Since the probability distribution of the series, satisfying the constraint that j_k occurs $p_j N$-times, is uniform we can use (D7),

$$I[p] = \ln \Omega[p], \tag{D10}$$

where the number of the allowed series,

$$\Omega[p] = \frac{N!}{\prod_j (N p_j)!}. \tag{D11}$$

Stirling's formula, $\ln n! \approx n \ln n - n$, allows us to write

$$\begin{aligned} I[p] &= N \ln N - N - N \sum_j p_j \ln N p_j + N \sum_j p_j \\ &= -N \sum_j p_j \ln p_j \end{aligned} \tag{D12}$$

for large $N \to \infty$. The missing information per symbol,

$$S[p] = \frac{I[p]}{N} = -\sum_j p_j \ln p_j = -\langle \ln p \rangle, \tag{D13}$$

is the expectation value of $\ln p$ up to a sign and is well defined for non-numeric random variables, too.

What is the minimal number of yes/no questions, N_Q, needed to identify the actual series if the distribution function is known? The optimally posed questions obviously split the possibilities into two equal parts, therefore

$$2^{N_Q} = \Omega[p] = e^{-N\sum_j p_j \ln p_j} \tag{D14}$$

and

$$N_q \ln 2 = \frac{\text{missing information}}{\text{symbol}}, \tag{D15}$$

the missing information of a symbol is proportional to the minimal number of questions needed to find its value.

5. Maximal entropy principle

Suppose that have some partial information about a random variable, expressed in terms of some expectation values. How to assign a probability distribution to this variable which is consistent with the constraint and contains as little additional information as possible? Suppose that a random event occurs N-times, $(x(t_1), \ldots, x(t_N))$, $x(t_j) \in \{x_1, \ldots, x_n\}$ and we know the average of the functions $f_k(x)$, $k = 1, \ldots, m$,

$$\frac{1}{N}\sum_j \boldsymbol{f}(x(t_j)) = \boldsymbol{F}. \tag{D16}$$

According to the maximal entropy principle (MAXENT) the optimal probability distribution $p(x|\boldsymbol{F})$ maximizes the missing information, $I[p]$, subject of the constraints

$$\sum_j p_j \boldsymbol{f}(x_j) = \boldsymbol{F}. \tag{D17}$$

The constraints are treated by means of Lagrange multipliers, by maximizing

$$S_F = -\sum_j p_j \ln p_j + (1-\lambda_0)(\sum_j p_j - 1) + \boldsymbol{\lambda}(\boldsymbol{F} - \sum_j p_j \boldsymbol{f}(x_j)) \tag{D18}$$

in the probability distribution $\{p_1, \ldots, p_n\}$ and the parameters λ_0, $\boldsymbol{\lambda}$. The extremal conditions for p_j,

$$0 = -\ln p_j - 1 - \lambda_0 + 1 - \boldsymbol{\lambda}\boldsymbol{f}(x_j), \tag{D19}$$

fixes the probability distribution,

$$p_j = e^{-\lambda_0 - \boldsymbol{\lambda}\boldsymbol{f}(x_j)}, \tag{D20}$$

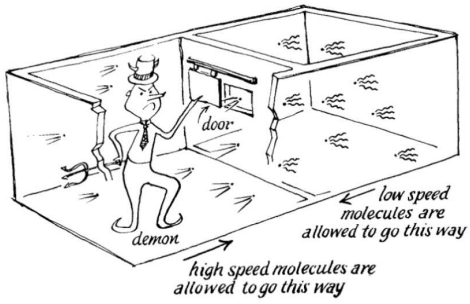


FIG. 10: Maxwell's demon after W. F. Angrist and L. G. Hepler, *Order and Chaos* (Basic Books, New York, 1967)

and the maximization in λ_0 yields the partition function,

$$\frac{\partial}{\partial \lambda_0} \; : \; 1 = e^{-\lambda_0} Z(\boldsymbol{\lambda}), \quad Z(\boldsymbol{\lambda}) = \sum_j e^{-\boldsymbol{\lambda} \boldsymbol{f}(x_j)} = e^{\lambda_0}. \tag{D21}$$

The maximization over $\boldsymbol{\lambda}$ gives the sum rules to express expectation values as the logarithmic derivatives of the partition function,

$$\frac{\partial}{\partial \boldsymbol{\lambda}} \; : \; \boldsymbol{F} = e^{-\lambda_0} \sum_j \boldsymbol{f}(x_j) e^{-\boldsymbol{\lambda} \boldsymbol{f}(x_j)} = \frac{1}{Z(\boldsymbol{\lambda})} \sum_j \boldsymbol{f}(x_j) e^{-\boldsymbol{\lambda} \boldsymbol{f}(x_j)} = -\frac{\partial \ln Z(\boldsymbol{\lambda})}{\partial \boldsymbol{\lambda}}. \tag{D22}$$

The value of the maximal entropy is

$$\begin{aligned} S_{max} &= -\sum_j p_j \ln p_j \\ &= \sum_j e^{-\lambda_0 - \boldsymbol{\lambda} \boldsymbol{f}(x_j)} [\lambda_0 + \boldsymbol{\lambda} \boldsymbol{f}(x_j)] \\ &= \lambda_0 + \boldsymbol{\lambda} \boldsymbol{F}. \end{aligned} \tag{D23}$$

6. Maxwell's demon

A relation between the thermodynamical entropy and information has bee suspected ever since James Clerk Maxwell proposed his demon as a counter example of thermodynamics in 1871. Imagine two containers, holding a gas at different temperature. The demon, Maxwell's small (internal physical laws ignored) and intelligent (capable of information treatment) creature is supposed to stand in the colder gas, beside a small windows (no mass and internal dynamics), separating two containers. Whenever a faster than the average gas molecule approaches the demon opens the window for a very short time and lets the particle to move into the warmer container. The second law of thermodynamics is violated in this manner.

Leo Szilárd has shown in 1929 that the second law can be saved by associating an appropriate entropy change to information gathering and processing, thereby linking entropy and information. The simplified argument in nutshell is the following: Let us take a single atom, equipped with an internal degree of freedom which can take two values, $y = 1, 2$ and place it into a system of two containers with open window. After thermalization the probability to find the atom in container j is $p_j = \frac{V_j}{V_1+V_2}$, $j = 1, 2$, V_j denoting the volume of the container. Now we let Maxwell's demon measure the value of y and work with the algorithm of placing the atom in container $j = y$ in equilibrium with the environment, along an isotherm. The decrease of (Boltzmann's) entropy if the atom is found in container j is $\Delta S_j = \ln \frac{V_j}{V_1+V_2} = \ln p_j$. Hence the average entropy change is $\sum_j p_j \ln p_j < 0$. The second law is rescued if there is an entropy production, s_j, associated to the measurement which finds the atom in container j and the inequality

$$\sum_j p_j(s_j + \ln p_j) \geq 0 \tag{D24}$$

is respected. An elementary argument[2] shows that this inequality follows if

$$\sum_j e^{-S_j} \leq 1. \tag{D25}$$

In particular, a demon, working in a reversible manner and producing the entropy $\Delta S = \ln 2$ remains in agreement with thermodynamics. The inequality (D24) amounts to the statement that the average entropy production of the measurement should exceed Shannon's information about the position of the atom in the containers, thereby balancing the thermodynamical entropy with information. A reversible demon, working with the uniform distribution, $p_1 = p_2 = \frac{1}{2}$, should produce the entropy which is equivalent with the gain of information.

The first reconciliation of Maxwell's demon and the second law of thermodynamics was achieved by Leon Brillouin in 1951 by noting that the demon is surrounded by the black body radiation of photons and need a higher temperature torch to perform the measurement. The information gathering process with such an object produces enough entropy to save the second law. A more general solution of the problem, posed by the demon, came from Rolf Landauer in 1961 by noting that the demon's memory has to be reset after each intervention and such an irreversible step alone produces enough entropy to restore the second law.

Appendix E: Density matrix

Gelason's theorem states that the mosg general probability assignement in a Hilbert space with at leats three dimensions is defined by the help of an operator ρ, called density matrix which acts

in the space of states. The probability to find the system in a normalised state $|\psi\rangle$ is

$$p_\psi = \langle\psi|\rho|\psi\rangle = \mathrm{Tr}[\rho|\psi\rangle\langle\psi|]. \tag{E1}$$

As a result, the the expectation value of an observable $A = \sum_n |n\rangle a_n \langle n|$ is given by

$$\bar{A} = \sum_n a_n p_{|n\rangle} = \sum_n a_n \mathrm{Tr}[\rho|n\rangle\langle n|] = \mathrm{Tr}[\rho A]. \tag{E2}$$

The density matrix possesses the following properties:

1. $\rho^\dagger = \rho$: Any operator can be written as the sum of a Hermitian and an anti-Hermitian piece, $\rho = \rho_h + \rho_{ah}$, with $\rho_h = \frac{1}{2}(\rho + \rho^\dagger)$ and $\rho_{ah} = \frac{1}{2}(\rho - \rho^\dagger)$. The probability $\mathrm{Tr}P_\psi\rho = \langle\psi|\rho|\psi\rangle$ is real $|\psi\rangle$ hence $\langle\psi|\rho|\psi\rangle = \langle\psi|\rho^\dagger|\psi\rangle$. This equation holds for an arbitrary vector $|\psi\rangle$ therefore $\rho_{ah} = 0$.

2. The density matrix is a positive operator because its expectation value in any state is non-negative, $\langle\psi|\rho|\psi\rangle = \mathrm{Tr}P_\psi\rho \geq 0$.

3. $\mathrm{Tr}\rho = 1$: The probability of the whole space of events, $\mathrm{Tr}\mathbb{1}\rho$ is unity.

4. The density matrix, being a Hermitian operator, is diagonalizable and can be written as

$$\rho = \sum_n |\psi_n\rangle PIN \langle\psi_n|, \tag{E3}$$

$\{|\psi_n\rangle\}$ being an orthonormal base. The eigenvalues are real, $0 \leq p_n$, and the diagonalization preserves the trace, $\sum_n p_n = 1$. The spectrum, $\{p_n\}$, can be interpreted as the probability of finding the system in one of the states, $|\psi_n\rangle$ since

$$\mathrm{Tr}A\rho = \sum_n p_n \langle\psi_n|A|\psi_n\rangle. \tag{E4}$$

5. The inequality

$$\mathrm{Tr}p^2 = \sum_n p_n^2 \leq \sum_n p_n = \mathrm{Tr}\rho \tag{E5}$$

becomes an equality only for pure states, $\rho = |\psi\rangle\langle\psi|$. The states with strict inequality are called mixed. The decomposition of the density matrix as a sum over pure state projectors is not unique, there are different systems of non-orthogonal states which yield the same density matrix.

Examples:

1. Spin states: The most general density matrix of a two-state system is

$$\rho = \frac{1}{2}(\mathbb{1} + \boldsymbol{p}\boldsymbol{\sigma}) \tag{E6}$$

where the Pauli-matrices are

$$\boldsymbol{\sigma} = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right). \tag{E7}$$

This corresponds to the mixture of two states with probabilities $\frac{1}{2}(1 \pm |\boldsymbol{p}|)$ and

$$\langle \boldsymbol{\sigma} \rangle = \mathrm{tr}\rho\boldsymbol{\sigma} = \boldsymbol{p}. \tag{E8}$$

Since $\mathrm{tr}\rho^2 = \frac{1+\boldsymbol{p}^2}{2}$, $|\boldsymbol{p}| \leq 1$, the equality belonging to pure states.

2. Canonical ensemble: The probability of finding a classical system, attached to a heat bath of temperature T and having the energy E is

$$p(E) = \frac{1}{Z} e^{-\frac{E}{k_B T}}, \quad Z = \sum_E e^{-\frac{E}{k_B T}}. \tag{E9}$$

The quantum ensemble assign the same probability to the stationary states, leading to the density matrix,

$$\rho = \frac{1}{Z} e^{-\frac{H}{k_B T}}, \quad Z = \mathrm{Tr} e^{-\frac{H}{k_B T}}. \tag{E10}$$

Appendix F: Time reversal

The time reversal implies the exchange of the initial and final conditions and the execution of the time reversal transformation on each physical quantity, $A(t)$, as $A(t) \to TA(t) = \tau_A A(-t)$, τ_A being the internal time parity. Note that ∂_t flips the sign of the parity, $\tau_{\partial_t A} = -\tau_A$, assuming that the latter is well defined. Since two time reversals, performed successively, leave the time arrow unchanged $\tau_A^2 = 1$ in classical physics. The time reversal should not mix imaginary components to a real quantity therefore τ_A is real and $\tau_A = \pm 1$.

The last two equations are not always valid in quantum mechanics where we need a more detailed construction of the time reversal transformation, revealing a further distinguishing feature of the time as opposed to the space. We start by noting that the physical states realize a ray-representation in the Hilbert space: The normalized vectors $|\psi\rangle$ and $e^{i\alpha}|\psi\rangle$, $\alpha \in \mathcal{R}$ give the same

averages thus represent the same state. Therefore the transformation $|\psi\rangle \to U|\psi\rangle$ is physically equivalent with $|\psi\rangle \to e^{i\alpha}U|\psi\rangle$ and the preservation of the scalar product, $\langle\psi|\phi\rangle = \langle U\psi|U\phi\rangle$, a precondition on any transformation to be elevated to the rank of a symmetry, can be relaxed to the preservation of the magnitude of the scalar product $|\langle\psi|\phi\rangle| = |\langle U\psi|U\phi\rangle|$.

Such a weakening of the unitarity widens the possibilities of representing symmetries in quantum mechanics. Wigner's theorem asserts that the invertible transformations of the linear space of the pure states onto themselves which preserve the transition probabilities, i.e. the absolute magnitude square of the scalar product, are either unitary or anti-unitary. An operator S is called linear or anti-linear if

$$S(a|\phi\rangle + b|\psi\rangle) = aS|\phi\rangle + bS|\psi\rangle, \tag{F1}$$

or

$$S(a|\phi\rangle + b|\psi\rangle) = a^*S|\phi\rangle + b^*S|\psi\rangle, \tag{F2}$$

respectively. The linear operator U is unitary if it is linear and

$$|\psi\rangle \to U|\psi\rangle = |\tilde{\psi}\rangle, \quad \langle\psi|\phi\rangle = \langle\tilde{\psi}|\tilde{\phi}\rangle. \tag{F3}$$

An anti-unitary operator A is an anti-linear operator and it satisfies

$$|\psi\rangle \to A|\psi\rangle = |\tilde{\psi}\rangle, \quad \langle\psi|\phi\rangle = \langle\tilde{\psi}|\tilde{\phi}\rangle^*. \tag{F4}$$

The anti-linear operators have few rather unattractive features, for instance they act only to the right in the bra-ket formalism,

$$\langle\psi|K_{\to}a|\phi\rangle = a^*\langle\psi|K|\phi\rangle \neq \langle\psi|_{\leftarrow}Ka|\phi\rangle = a\langle\psi|K|\phi\rangle, \tag{F5}$$

therefore one applies them in the wave function formalism.

The time reversal, $T|\psi(t)\rangle = |\psi(t)^T\rangle$, is anti-linear in quantum mechanics to preserve the canonical commutation relation. The action of the time reversal on the wave function of a state with positive internal time parity is defined as $T\psi(\boldsymbol{x}) = \psi^*(\boldsymbol{x})$ in the coordinate representation. The application of this rule to $\psi_{\boldsymbol{p}}(\boldsymbol{x}) = \langle\boldsymbol{x}|\boldsymbol{p}\rangle = e^{\frac{i}{\hbar}\boldsymbol{x}\boldsymbol{p}}$ yields the transformation

$$T\psi_{\boldsymbol{p}}(\boldsymbol{x}) = Te^{\frac{i}{\hbar}\boldsymbol{x}\boldsymbol{p}} = e^{-\frac{i}{\hbar}\boldsymbol{x}\boldsymbol{p}} = \psi_{-\boldsymbol{p}}(\boldsymbol{x}), \tag{F6}$$

which in turn gives

$$T\tilde{\psi}(\boldsymbol{p}) = T\int d^3x e^{-\frac{i}{\hbar}\boldsymbol{x}\boldsymbol{p}}\psi(\boldsymbol{x}) = \int d^3x e^{\frac{i}{\hbar}\boldsymbol{x}\boldsymbol{p}}\psi^*(\boldsymbol{x}) = \psi^*(-\boldsymbol{p}). \tag{F7}$$

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[1] The justification of this point requires the proper, simultaneous treatment of the three steps of the measuring process, considered sequentially here.

[2] The minimization of (D24) in p_j yields $s_1 - s_2 + \ln p_1 - \ln p_2 = 0$. Let us introduce $\lambda = s_j + \ln p_j$ and write $p_j = e^{\lambda - s_j}$. The inequality $\lambda e^{\lambda} \sum_j e^{-s_j} \geq 0$ which follows from (D24) requires $\lambda \geq 0$. The sum rule $\sum_j p_j = 1$ implies $\sum_j e^{-s_j} = e^{-\lambda}$. This equation and the previous two inequalities yield (D25).