The arrow of time

Janos Polonyi
University of Strasbourg
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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, existing in classical physics only, and one expects that the time and the space have 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

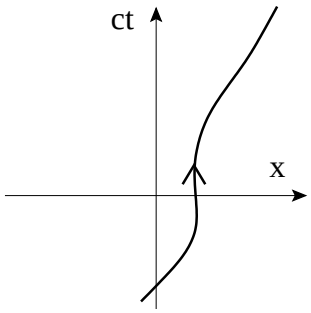


FIG. 1: The world line representation of the motion of a point particle in relativity.

for the world line of a particle. The Lorentz transformation, expressing a symmetry of all known 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 gains the superficial impression that space and time are somehow equivalent. 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. Feature 2. above is essential here since the measurement of the time by periodic motion requires a counter with a memory, requiring irreversibility. In other words, the time possesses a direction by definition.

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.

One can extract two time arrows:

1. τ_d: A dynamical time arrow is defined by the irreversibility: The dynamics is stable in the direction of the dynamical time arrow and is self-accelerating and unstable in the opposite

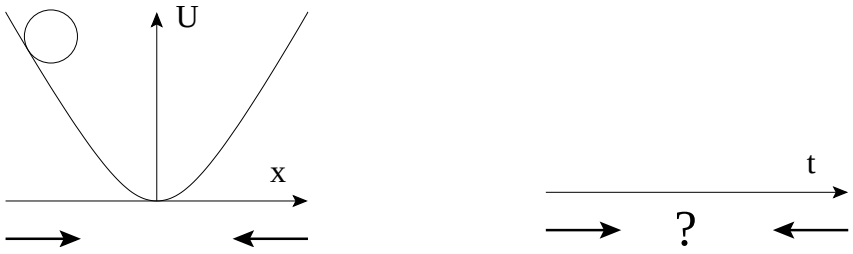


FIG. 2: The direction of the displacement in space is not unique, as opposed to the time.

direction. The dynamical time arrow is encoded by the time reversal invariance breaking terms of the equations of motion.

2. τ_c: The causal time arrow can be observed by considering two copies of the system in question which are sufficiently well separated to exclude the interaction between them by rearranging 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. The causal time arrow is implemented in our calculations by imposing the initial ($\tau_c = 1$) or the final conditions ($\tau_c = -1$), the time flows away from the auxiliary conditions. One can construct models, defined by using both initial and final conditions, which do not possess causal time arrow. The causal time arrow can be defined even if the equations of motion are time reversal invariant.

A number of questions arise in a natural manner:

- How can one recognize the presence of a time arrow, i.e. the breakdown of the time reversal invariance, 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.

- The experiences suggest that macroscopic systems follow deterministic laws and in particular possess a causal time arrow. It is natural to raise the question whether Nature realizes the mathematical possibility of systems with no causal time arrow. In other words, do all the macroscopic physical system has a 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 fundamental interactions are time reversal invariant and leave the time unoriented. (To be precise one should add that the weak interaction assigns a time arrow but it turns out to be too weak 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?

This lecture deals mainly with the last question and few examples of the time arrows, followed by the technical key words to be discussed later, are the following:

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 piece of paper with a fountain pen. The writing is a stable carrier of information because the ink diffuses into the papers. Seeing this backward in a movie the ink is found to be suck in by the pen from the paper. (irreversibility)

3. Quantum time arrow: A photon, propagating in the assumed vacuum of the interstellar space is in a state of a plane wave and has no position whatsoever. It interacts with a dust particle and at the instant of its absorption it acquires a position, that of the elementary particle of the dust, absorbing it. This is called the collapse of the wave function of the photon (and the elementary particle in question), a sudden change from an extended form to a localized one. Seeing backward on a video recording one witnesses a creation of the photon at a given position in space. This always leads to spherical waves and only later filtering processes can narrow it down to a plane wave. (loss of informations 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.

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. This is sufficient in classical physics but we need a different description of the electromagnetic interaction in the quantum domain.

The reason is that each the wave functions, $\psi(x)$ and $e^{i\chi}\psi(x)$, represent the same physical state. Such a global, space-time independent phase symmetry must be extended to a symmetry under local gauge transformation,

$$\psi(x) \to e^{ie\chi(x)}\psi(x), \tag{2}$$

in relativistic theories to respect causality. The derivative of the wave function transforms in an inhomogeneous manner, $\partial_\mu\psi(x) \to [\partial_\mu + ie\partial_\mu\chi(x)]\psi(x)$, under gauge transformation. To restore the symmetry the partial derivatives are replaced by the covariant derivative, $D_\mu\psi(x) = [\partial_\mu - eA_\mu(x)]\psi(x)$, everywhere in the equations. The gauge transformation acts on the gauge field, $A_\mu(x)$, as

$$A_\mu(x) \to A_\mu(x) - \partial_\mu\chi(x), \tag{3}$$

to restore the simple, homogeneous transformation of the covariant derivative of the wave function,

$$D_\mu\psi(x) = [\partial_\mu - eA_\mu(x)]\psi(x) \to e^{ie\chi(x)}D_\mu\psi(x)\partial\psi(x), \tag{4}$$

valid for partial derivative and global phase transformation, $\partial_\mu\psi(x) \to e^{ie\chi(x)}\partial_\mu\psi(x)$. The gauge field, $A_\mu(x) = (\phi(x), -\boldsymbol{A}(x))$, introduced in such a manner is responsible of the electromagnetic interaction.

The third Maxwell equation suggest the definition

$$\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A} \tag{5}$$

of the magnetic field which brings the fourth equation into the form

$$0 = \boldsymbol{\nabla}\times\left(\boldsymbol{E} + \frac{1}{c}\partial_t\boldsymbol{A}\right), \tag{6}$$

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

$$\boldsymbol{E} = -\boldsymbol{\nabla}\phi - \frac{1}{c}\partial_t\boldsymbol{A}. \tag{7}$$

Note that the magnetic and electric fields, defined by eqs. (5)-(7), remain the same if the gauge potentials ϕ and $\boldsymbol{A}$ are modified according to the gauge transformation

$$\phi(x) \to \phi(x) - \frac{1}{c}\partial_t\chi(x), \quad \boldsymbol{A}(x) \to \boldsymbol{A}(x) - \boldsymbol{\nabla}\chi(x). \tag{8}$$

This transformation can be written in a more compact form (3) 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 condition,

$$\frac{1}{c}\partial_t\phi + \boldsymbol{\nabla}\boldsymbol{A} = 0. \tag{9}$$

The first two, inhomogeneous Maxwell equation read as

$$\begin{aligned} 4\pi\rho &= -\boldsymbol{\nabla}\left(\boldsymbol{\nabla}\phi + \frac{1}{c}\partial_t\boldsymbol{A}\right) = \left(\frac{1}{c^2}\partial_t^2 - \Delta\right)\phi = \Box\phi, \\ \frac{4\pi}{c}\boldsymbol{j} &= \frac{1}{c}\partial_t\left(\boldsymbol{\nabla}\phi + \frac{1}{c}\partial_t\boldsymbol{A}\right) + \boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\boldsymbol{A} = \left(\frac{1}{c^2}\partial_t^2 - \Delta\right)\boldsymbol{A}, \end{aligned} \tag{10}$$

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

$$\Box A^\mu = \frac{4\pi}{c}j^\mu. \tag{11}$$

A. Radiation field

We assume that the electric current, $j^\mu(x)$, is non-vanishing in a finite time interval only and seek the induced electromagnetic field. To obtain a unique solution of eq. (11) 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 (11) 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.

The inhomogeneous solutions can be written in the form,

$$\begin{aligned} A^\mu_{ih}(x) &= \frac{4\pi}{c}\int d^4y \overset{r}{D^a}(x-y)j^\mu(y), \\ &= \frac{1}{c}\int d^4y \frac{\delta(x^0 - y^0 \mp |\boldsymbol{x}-\boldsymbol{y}|)j^\mu(y)}{|\boldsymbol{x}-\boldsymbol{y}|}, \\ &= \frac{1}{c}\int d^3y \frac{j^\mu(x^0 \mp |\boldsymbol{x}-\boldsymbol{y}|, \boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}, \end{aligned} \tag{12}$$

by the help of the retarded and advanced Green's functions, obtained in appendix B30 since $\overset{r}{D^a}(x) = 0$ for $\mp x^0 > 0$. This expression shows clearly the retarded (advanced) feature of the

solution, defined by the initial (final) condition. The radiation, defined as the field, generated by the external source,

$$A_{rad} = A_{out} - A_{in} = 2A^f, \tag{13}$$

is given by the far field Green's function,

$$A^{\mu}_{rad}(x) = \frac{8\pi}{c} \int dy D^f(x-y) j^{\mu}(y) \tag{14}$$

c.f. eq. (B31).

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, $D^{\overset{r}{a}}(x^0, \boldsymbol{x}) \neq D^{\overset{r}{a}}(-x^0, \boldsymbol{x})$. 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 obviouisly 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 continuous symmetries of a closed system of classical particles restrict the equations of motions. A subsystem of a closed system usually looses the symmetries of the full system owing to the interaction with the environment. Such a sub-system is called open and its equations of motion are non-conservative and rather complicated. The following two features render the detailed dynamical treatment of the large, macroscopic systems difficult:

1. The large systems can not be isolated from their environment. It is shown in this section the interactions with the environment can generate a directed time for open systems.

2. Avogadro's number, 6×10^{23} is quite large, the macroscopic systems possess an exceedingly large number of degrees of freedom. Te discussion of the impact of this complication on the time arrow problem is left for 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,

$$\ddot{x}(t) = F(x(t), y(t)), \quad \ddot{y}(t) = G(x(t), y(t)), \tag{15}$$

and the auxiliary conditions, chosen as initial conditions,

$$x(t_i) = x_i, \quad \dot{x}(t_i) = v_i, \quad y(t_i) = y_i, \quad \dot{y}(t_i) = u_i. \tag{16}$$

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, $y[t, x, y_i, u_i]$, back into the system equation of motion. The result is a nonlocal equation of motion,

$$\ddot{x}(t) = F(x(t), y[t, x, y_i, u_i]), \tag{17}$$

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, nonlocal terms of the equation of motion, usually approximated by local expressions, obtained within the framework of the expansion in the time derivative. The environment auxiliary conditions break the time reversal invariance of the equation of motion and generate a direction for the time. Suppose that we make a video recording of the dynamics of the system. Though one sees neither the environment nor its time arrow in the recording our experience about the direction of the time of the effective dynamics allows us to recognise that scene, seen on the backward played video recording is unusual, the system and the environment having 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

$$\begin{aligned} L &= \frac{m}{2}\dot{x}^2 - \frac{m\omega_0^2}{2}x^2 - jx + \sum_n \left(\frac{m}{2}\dot{y}_n^2 - \frac{m\omega_n^2}{2}y_n^2 - g_n x y_n\right) \\ &= \frac{m}{2}\dot{x}^2 + \left(\frac{m\omega_0^2}{2} - \sum_n \frac{g_n^2}{2m\omega_n^2}\right)x^2 - jx + \sum_n \left[\frac{m}{2}\dot{y}_n^2 - \frac{m\omega_n^2}{2}\left(y_n + \frac{g_n x}{m\omega_n^2}\right)^2\right], \end{aligned} \tag{18}$$

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,

$$x(\omega) = \int dt e^{i\omega t} x(t), \tag{19}$$

in the frequency space as

$$m\omega^2 y_n(\omega) = m\omega_n^2 y_n(\omega) + g_n x(\omega), \tag{20}$$

can easily be solved,

$$y_n(\omega) = \frac{g_n x(\omega)}{m(\omega^2 - \omega_n^2)} = \tilde{D}_n(\omega) g_n x(\omega). \tag{21}$$

The environment Green's function,

$$\tilde{D}_n(\omega) = \frac{1}{m[(\omega + i\epsilon_e)^2 - \omega_n^2]} \tag{22}$$

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,

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

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

$$\tilde{\Sigma}(\omega) = \sum_n g_n^2 D_n(\omega) = \sum_n \frac{g_n^2}{m} \frac{1}{(\omega + i\epsilon_e)^2 - \omega_n^2}, \tag{24}$$

is used to define the effective Green's function,

$$\tilde{D}_{eff}(\omega) = \frac{1}{m[(\omega + i\epsilon_s)^2 - \omega_0^2] - \tilde{\Sigma}(\omega)}. \tag{25}$$

The system trajectory, corresponding to a given external source,

$$x(t) = \int_{-\infty}^{\infty} dt' D_{eff}(t - t') j(t'), \tag{26}$$

satisfies the effective equation of motion,

$$\tilde{D}_{eff}^{-1} x(\omega) = m \left[(\omega + i\epsilon_s)^2 - \omega_0^2 - \sum_n \frac{g_n^2}{m} \frac{1}{(\omega + i\epsilon_e)^2 - \omega_n^2} \right] x(\omega) = j(\omega), \tag{27}$$

which is non-local in time,

$$m\ddot{x}(t) = -m\omega_0^2 x(t) + \mathrm{sign}(\epsilon_e) \sum_n \frac{g_n^2}{m^2 \omega_n} \int_{-\infty}^{\infty} dt' \Theta(\mathrm{sign}(\epsilon_e)(t - t')) \sin \omega_n (t - t') x(t') - j(t). \tag{28}$$

C. Spectral function

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

$$\rho(\Omega) = \sum_n \frac{g_n^2}{2m\omega_n} \delta(\omega_n - \Omega), \tag{29}$$

which allows us to write

$$\tilde{\Sigma}(\omega) = \int d\Omega \frac{2\rho(\Omega)\Omega}{(\omega + i\epsilon_e)^2 - \Omega^2}. \tag{30}$$

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

$$\rho(\Omega) = \Theta(\Omega) \frac{g^2 \Omega}{m\Omega_D(\Omega_D^2 + \Omega^2)}, \tag{31}$$

yielding

$$\begin{aligned}
\tilde{\Sigma}(\omega) &= \frac{g^2}{m\Omega_D} \int d\Omega \Theta(\Omega) \frac{\Omega}{\Omega_D^2 + \Omega^2} \frac{2\Omega}{(\omega + i\epsilon_e)^2 - \Omega^2} \\
&= -\frac{g^2}{m\Omega_D} \int d\Omega \frac{\Omega^2}{(\Omega + i\Omega_D)(\Omega - i\Omega_D)(\Omega - \omega - i\epsilon_e)(\Omega + \omega + i\epsilon_e)} \\
&= -\frac{g_e^2}{m\Omega_D} 2\pi i \left[\frac{\Omega_D^2}{2i\Omega_D(\omega^2 + \Omega_D^2)} + \mathrm{sign}(\epsilon_e) \frac{\omega^2}{(\omega^2 + \Omega_D^2) 2(\omega + i\epsilon_e)} \right] \\
&= -\frac{g^2 \pi}{m\Omega_D} \frac{\Omega_D + i\mathrm{sign}(\epsilon_e)\omega}{\omega^2 + \Omega_D^2} = -\frac{\pi g^2}{m\Omega_D(\Omega_D - i\mathrm{sign}(\epsilon_e)\omega)}
\end{aligned} \tag{32}$$

and

$$\tilde{D}_{eff}(\omega) = \frac{1}{m[(\omega + i\epsilon_s)^2 - \omega_0^2] + \frac{\pi g^2}{m\Omega_D(\Omega_D - i\mathrm{sign}(\epsilon_e)\omega)}}. \tag{33}$$

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

$$\tilde{D}_{eff}(\omega) = \frac{1}{m(\omega^2 - \omega_0^2) + \frac{\pi g^2}{m\Omega_D(\Omega_D - i\mathrm{sign}(\epsilon_e)\omega)}}. \tag{34}$$

The effective equation of motion,

$$\tilde{D}_{eff}^{r-1}x(\omega) = m\left[\omega^2 - \omega_0^2 + \frac{\pi g^2}{m^2\Omega_D(\Omega_D - i\mathrm{sign}(\epsilon_e)\omega)}\right]x(\omega) = j(\omega), \tag{35}$$

is a non-local, integro-differential equation in time,

$$\begin{aligned} m\ddot{x}(t) &= -m\omega_0^2 x(t) + i\mathrm{sign}(\epsilon_e)\frac{g^2}{2m\Omega_D}\int_{-\infty}^{\infty} d\omega dt' \frac{e^{-i\omega(t-t')}}{\omega + i\mathrm{sign}(\epsilon_e)\Omega_D}x(t') - j(t) \\ &= -m\omega_0^2 x(t) - i\frac{\pi g^2}{m\Omega_D}\int_{-\infty}^{\infty} dt'\theta(\mathrm{sign}(\epsilon_e)(t-t'))e^{-\Omega_D(t-t')}x(t') - j(t), \end{aligned} \tag{36}$$

with a memory time scale, $\tau_{mem} = 1/\Omega_D$. The effective equation of motion reduces to

$$m[(\omega + i\epsilon_s)^2 - \omega_{eff}^2 + i\mathrm{sign}(\epsilon_e)\nu\omega]x(\omega) = j(\omega), \tag{37}$$

for slow motion, $\omega \to 0$, containing the effective frequency, $\omega_{eff}^2 = \omega_0^2 - \frac{\pi g^2}{m^2\Omega_D^2}$, and the friction constant, $\nu = \frac{\pi g^2}{m^2\Omega_D^3}$. The real time form,

$$\ddot{x}(t) = -\omega_{eff}^2 x(t) - \mathrm{sign}(\epsilon_e)\nu\dot{x}(t) - j(t), \tag{38}$$

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.

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. The potential energy in the second line of eqs. (18) is a positive quadratic form hence the normal mode spectrum is real. As a result, the effective Green's function, (27), has pole in the appropriate half plane of the complex frequency and is therefore causal for $\mathrm{sign}(\epsilon_s) = \mathrm{sign}(\epsilon_e)$, c.f. Figs. 3 (a) and (f).

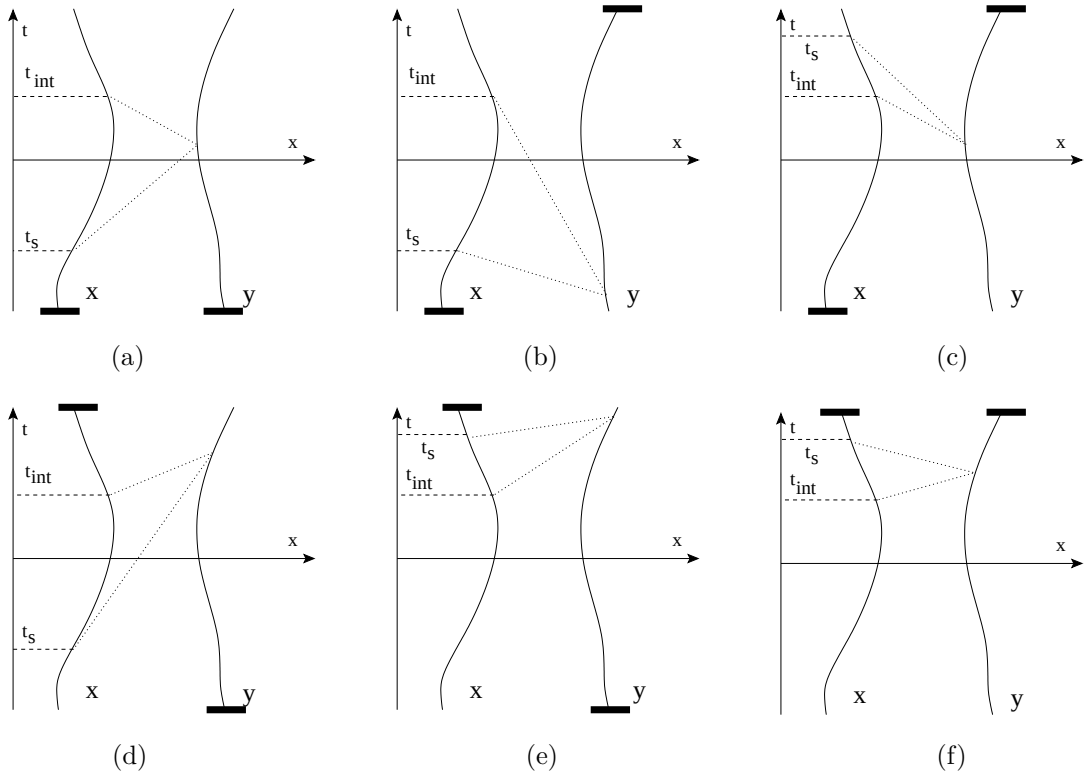
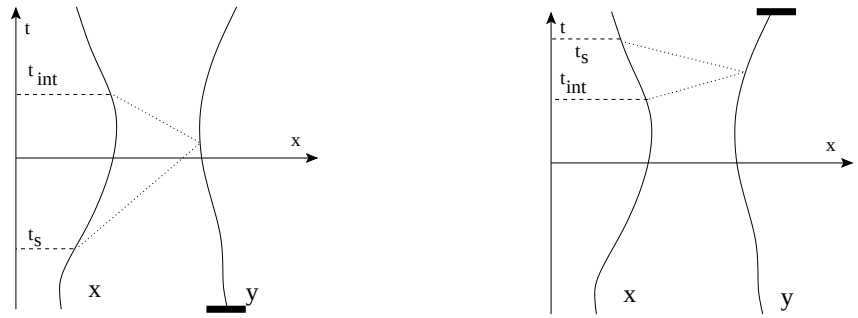


FIG. 3: The causal structure of the self interaction of the observed system, mediated by an environment with discrete spectrum. The system interacts at time t_{int} with itself when it is at the source time t_s. The auxiliary conditions are imposed at the initial or final time, denoted by a short, fat horizontal line. (a): $\epsilon_s > 0$, $\epsilon_e > 0$, (b): $\epsilon_s > 0$, $\epsilon_e < 0$, $t_{int} > t_s$, (c): $\epsilon_s > 0$, $\epsilon_e < 0$, $t_{int} < t_s$, (d): $\epsilon_s < 0$, $\epsilon_e > 0$, $t_{int} > t_s$, (e): $\epsilon_s < 0$, $\epsilon_e > 0$, $t_{int} < t_s$, (f): $\epsilon_s < 0$, $\epsilon_e < 0$.

There are poles on both half plane for $\mathrm{sign}(\epsilon_s) = -\mathrm{sign}(\epsilon_e)$ there is no definite order between the interaction and the sourc time on Figs. 3 (b), (c),(d) and (e) and the effective interaction is acausal. It is worthwhile keeping in mind that there is another way acausality may arise in a formal calulation. 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 (37). The distinguishing feature of dissipative forces is that they pass the environment time arrow to the



(a) (b)

FIG. 4: The causal structure of the self interaction of an irreversible system, in the presence of an enivronment with continuous spectrum without gap. 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 due to the dissipative forces. (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 (a) and (b), c.f. eq. (B19).

E. Broken time reversal invariance and irreversibility

A 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,

$$H = \frac{m}{2}\dot{x}^2 + \frac{m\omega_0^2}{2}x^2 + \sum_n \left(\frac{m}{2}\dot{y}_n^2 + \frac{m\omega_n^2}{2}y_n^2 + g_n x y_n\right), \tag{39}$$

can be expressed in terms of the system coordinate,

$$\begin{aligned}
H(t) &= \frac{m}{2}\dot{x}^2(t) + \frac{m\omega_0^2}{2}x^2(t) + \sum_n g_n^2\Bigg[\frac{m}{2}\left(\int dt'\partial_t D_n^r(t-t')x(t')\right)^2 \\
&\quad + \frac{m\omega_n^2}{2}\left(\int dt' D_n^r(t-t')x(t')\right)^2 + x(t)\int dt' D_n^r(t-t')x(t')\Bigg] \\
&= \frac{m}{2}\dot{x}^2(t) + \frac{m\omega_0^2}{2}x^2(t) + \sum_n g_n^2\Bigg\{[x(t)\int dt' D_n^r(t-t')x(t') \\
&\quad + \frac{m}{2}\int dt'dt'' x(t')[\partial_t D_n^r(t-t')\partial_t D_n^r(t-t'') + \omega_n^2 D_n^r(t-t')D_n^r(t-t'')]x(t'')\Bigg\} \\
&= \frac{m}{2}\dot{x}^2(t) + \frac{m\omega_0^2}{2}x^2(t) + \sum_n \frac{g_n^2}{m}\Bigg[-x(t)\int_{-\infty}^{t} dt' \frac{\sin\omega_n(t-t')}{\omega_n}x(t') \\
&\quad + \frac{1}{2}\int_{-\infty}^{t} dt'dt'' x(t')[\cos\omega_n(t-t')\cos\omega_n(t-t'') + \sin\omega_n(t-t')\sin\omega_n(t-t'')]x(t'')\Bigg].
\end{aligned} \tag{40}$$

To trace down the energy, absorbed by the mode y_n, implies the resolution of the amplitude of an oscillation with frequency ω_n and requires an observation time, $t_{obs} \gg 1/\omega_n$. This is finite if

there is a gap in the excitation spectrum, $\omega_n > \Delta\omega > 0$ and we can resolve each mode in the total energy, finding the system conservative despite the broken time reversal invariance.

Irreversibility may result from a soft environment which can be excited at arbitrarily low frequencies. In fact, a condensation point of the environment excitation spectrum at vanishing frequency indicates the presence of environment excitation modes with arbitrarily long time scale. No finite amount of time is sufficient in that case to resolve the environment modes which are relevant for the reconstruction of the system energy. Since the heat capacity of a soft environment diverges in the thermodynamical limit the unresolved environment modes serve as a sink for the system energy and generate dissipative forces.

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 reproducibility: 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 informations 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 thermo-

dynamical 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,

$$E = \langle H \rangle = \sum_n p_n E_n \tag{41}$$

whose change in an infinitesimal time,

$$\delta E = \delta Q + \delta W, \tag{42}$$

is the sum of two terms. The first,

$$\delta W = \sum_n p_n \delta E_n, \tag{43}$$

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,

$$\delta Q = \sum_n \delta p_n E_n, \tag{44}$$

denotes the energy received by the uncontrollable channels from the undobserved environment and is called heat. One recognizes in (42) 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,

$$S_{Cl} = \int \frac{\delta Q}{T}, \tag{45}$$

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,

$$\int_A^B \frac{\delta Q}{T} \leq S_{Cl}(B) - S_{Cl}(A), \tag{46}$$

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, (45), Boltzmann's expression,

$$S_B = \ln \frac{\Omega}{\Omega_0}, \tag{47}$$

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

$$S_G = -\int d^{3N}pd^{3N}qp(\boldsymbol{p},\boldsymbol{q}) \ln p(\boldsymbol{p},\boldsymbol{q}), \tag{48}$$

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 (47) and (48) 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 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 reproducibility of the thermodynamical laws makes the entropies (47) and (48), 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 (47) and (48).

The Gibbs entropy is obviously equivalent with the entropy, found by maximizing the missing information, (D18). 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 $1-\epsilon$,

$$\int_{\Sigma(\Phi)} d^{3N}pd^{3N}qp(\boldsymbol{p},\boldsymbol{q}) = 1-\epsilon \tag{49}$$

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

$$\Omega_N(\Sigma(\Phi),\epsilon) = \int_{\Sigma(\Phi)} d^{3N}pd^{3N}q, \tag{50}$$

approaches the Gibbs entropy in the thermodynamical limit,

$$\lim_{N\to\infty} \frac{\ln \frac{\Omega_N(\Sigma(\Phi),\epsilon)}{\Omega_0}}{N} = -\int d^{3N}pd^{3N}qp(\boldsymbol{p},\boldsymbol{q})\ln p(\boldsymbol{p},\boldsymbol{q}), \tag{51}$$

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

D. Second law and reproducibility

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

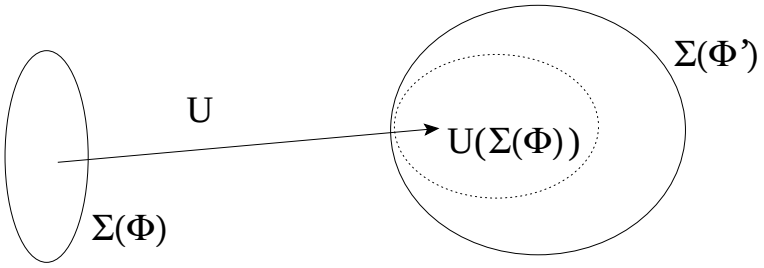


FIG. 5: The second law of thermodynamics: phase space volume of a macro state can not decrease during reproducible changes $\Phi_i \to \Phi_f$ of the thermodynamic variables.

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 full set of microscopic equations of motion with couplings to the environment ignored. Reproducibility is the inclusion

$$U_{t_f,t_i}(\Sigma(\Phi_i)) \subset \Sigma(\Phi_f), \tag{52}$$

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

$$\Omega(\Sigma(\Phi_f)) = \Omega(U_{t_f,t_i}(\Sigma(\Phi_i))) \tag{53}$$

where $\Omega(\Sigma(\Phi))$ denotes the volume of the macro state in the phase space, the inequality,

$$\Omega(\Sigma(\Phi_i)) \leq \Omega(\Sigma(\Phi_f)), \tag{54}$$

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

$$S(\Phi_i) = \ln \frac{\Omega(\Sigma(\Phi_i))}{\Omega_0} \leq \ln \frac{\Omega(\Sigma(\Phi_f))}{\Omega_0} = S(\Phi_f). \tag{55}$$

The inequalities (52) and (55) become equality for reversible reproducible processes.

One might think that the second law of thermodynamics, applied to isolated systems, implies a dynamical 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.

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. (42) and the entropy characterizes the latter.

The thermodynamical equation, (45), can be obtained by the help of Shannon's entropy,

$$\begin{aligned} \delta S &= \delta(-\sum_n p_n \ln p_n) \\ &= -\sum_n (\delta p_n) \ln p_n \\ &= \frac{1}{T} \sum_n E_n \delta p_n \\ &= \frac{\delta Q}{T} \end{aligned} \tag{56}$$

where the relation $\sum_n \delta p_m = 1$ was used in the second equation, the canonical probability distribution (D15) is used in the second third equation and finally, the last line follows from Eq. (44).

This equation, written in the form,

$$\frac{\delta Q}{T} = d \ln \Omega = \frac{d\Omega}{\Omega}, \tag{57}$$

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 enviornment) 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 estabilshing 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 mangitude 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

$$e^{-\frac{i}{\hbar}H_m t_m}|\phi_{k_i}\rangle \otimes |\chi_{\ell_i}\rangle = \sum_{k\ell} c^{k\ell}_{k_i\ell_i}|\phi_k\rangle \otimes |\chi_\ell\rangle, \tag{58}$$

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

$$e^{-\frac{i}{\hbar}H_m t_m}|\psi_i\rangle = \sum_{kk_i\ell\ell_i} \psi^{k_i\ell_i} c^{k\ell}_{k_i\ell_i}|\phi_k\rangle \otimes |\chi_\ell\rangle. \tag{59}$$

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,

$$e^{-\frac{i}{\hbar}(H_A+H_e+H_{Ae}}|\chi_{\ell_i}\rangle \otimes |\eta_{m_i}\rangle = \sum_{\ell m} d^{\ell m}_{\ell_i m_i}|\chi_\ell\rangle \otimes |\eta_m\rangle. \tag{60}$$

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

$$e^{-\frac{i}{\hbar}(H_A+H_e+H_{Ae}}|\chi_{\ell_i}\rangle \otimes |\eta_{m_i}\rangle = \sum_n d_n|\chi_n\rangle \otimes |\eta_n\rangle, \tag{61}$$

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,

$$\rho_A = \sum_{nn'} d_n d^*_{n'}\langle\eta_{n'}|\eta_n\rangle|\chi_n\rangle\langle\chi_{n'}|, \tag{62}$$

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

$$\mathrm{Tr}_A[A\rho_A] = \sum_{nn'} d_n d^*_{n'}\langle\eta_{n'}|\eta_n\rangle\langle\chi_{n'}|A|\chi_n\rangle. \tag{63}$$

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

$$\langle\chi|A|\chi\rangle = \sum_{nn'} d_n d^*_{n'}\langle\chi_{n'}|A|\chi_n\rangle, \tag{64}$$

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. (64) 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,

$$\langle \theta_1 | \theta_2 \rangle \approx (1 - c\Delta\theta)^N \approx e^{-cN\Delta\theta}, \tag{65}$$

$N \sim N_{Av} = 6 \cdot 10^{23}$ 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,

$$|\psi\rangle\langle\psi| \to \sum_n p_n |\psi_n\rangle\langle\psi_n|, \tag{66}$$

since the reduced density matrix, being Hermitian, is diagonalizable, and the quantum mechanical expectation value, $\langle \psi_n | A | \psi_n \rangle$, appears in (63) 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 informations, 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,

$$\rho_A = \sum_{k\ell\ell' m} \Psi_{k\ell m} \Psi^*_{k\ell' m} |\chi_\ell\rangle\langle\chi_{\ell'}|. \tag{67}$$

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

$$\rho_\ell = \frac{P_\ell \rho P_\ell}{Tr_s[P_\ell \rho P \ell]} = P_\ell, \tag{68}$$

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, (67), collapses onto a simple one, (68). 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 theorems used to calculate the Fourier integrals of the Green's functions is given below.

1. Cauchy-Riemann condition

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

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

implies quite strict properties owing to the complex nature of the difference, h, expressed by the Cauchy-Riemann equation. In fact, the equivalence of the derivative, calculated for real and purely imaginary h,

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

for real η gives the equation

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

when the parametrization $f = f_1 + if_2$ and $z = z_1 + iz_2$ is used. The result is the Cauchy-Riemann condition,

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

The differentiable functions are called holomorphic. Furthermore, a function, $f(z)$, is called analytic at z_0 with a radius of convergence r if the convergence

$$\lim_{N\to\infty} \sum_{n=1}^{N} a_n (z - z_0)^n = f(z) \tag{A5}$$

for $|z - z_0| < r$ is absolute and uniform. The order of integration and summation can be interchanged in this case.

2. Cauchy's theorem

Let U be a simply connected open set of the complex plane (a connected set is simply connected if any closed continuous loop, γ, can be continuously deformed to a point without leaving the domain) and $f(z)$ holomorphic on U. Cauchy's theorem states that the integral of $f(z)$ over γ in U is vanishing,

$$\oint_\gamma dz f(z) = 0. \tag{A6}$$

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

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

The application of this and the Cauchy-Riemann equations to the real and the imaginary part of (A7) yields

$$\oint_\gamma dz f(z) = -\int_D dz_1 dz_2 \left(\frac{\partial f_2}{\partial z_1} + \frac{\partial f_1}{\partial z_2} \right) + i \int_D dz_1 dz_2 \left(\frac{\partial f_1}{\partial z_1} - \frac{\partial f_2}{\partial z_2} \right) = 0. \tag{A10}$$

3. Residue theorem

The residue of a function $f(z)$ at z_0 is $Res f(z_0) = \lim_{z \to z_0} (z - z_0) f(z)$ if the limit exist. The residue is vanishing for homomorphic 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 $2\pi i$,

$$\oint_\gamma dz f(z) = 2\pi i \sum_{n=1}^{N} \nu_\gamma(z_n) Res f(z_n), \tag{A11}$$

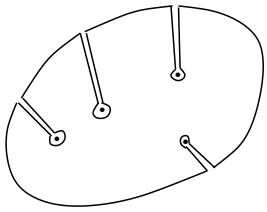


FIG. 6: The deformation of a closed integration contour by excluding the singularities.

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

$$\nu(z) = \frac{1}{2\pi i} \oint_\gamma dz' \frac{1}{z'-z}, \tag{A12}$$

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

$$\begin{aligned} \nu(z) &= \frac{1}{2\pi i} \int_0^{2\pi} d\alpha \frac{(\frac{dr}{d\alpha} + ir\frac{d\phi}{d\alpha})e^{i\phi}}{re^{i\phi}} \\ &= \frac{1}{2\pi i} \int_0^{2\pi} d\alpha \frac{d\ln r}{d\alpha} + \frac{1}{2\pi} \int_0^{2\pi} d\alpha \frac{d\phi}{d\alpha}. \end{aligned} \tag{A13}$$

The first integral is vanishing owing to the periodicity of the length parameter, $r(0) = r(2\pi)$, making ν an integer and 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. (A11) 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. 6

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

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

Since the right hand side plays the role of the identify operator on the space of time-dependent functions,

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

we have $G = L^{-1}$ and can solve our equation by writing,

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

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, $L(\partial_t)\phi(t) = 0$.

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

- The null-space consists of the solution of the equation of motion without external source, it contains the 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, $L = L^s + L^a$, $\overset{s}{L^a} = (L \pm L^{\rm tr})/2$, 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

$$x(t) = \int d\lambda x_\lambda \phi_\lambda(t) \tag{B5}$$

  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, $j_0 = 0$. This is an unacceptable restriction.

These problems can be avoided by imposing some auxiliary conditions on the solutions. We follow this procedure by starting from a formal, mathematical point, the removal of the null space of the equation of motion, the modification, $L \to L_\epsilon = L + i\epsilon$, which renders the Green's function well defined and perform the limit $\epsilon \to 0$ at the end of the calculation. We manage to break the invariance under time reversal, $L \to L^{*\rm tr}$, for any finite ϵ and we come back to this issue after the limit, $\epsilon \to 0$ has been taken.

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,

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

yieds immediately the Fourier transform and its inverse.

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,

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

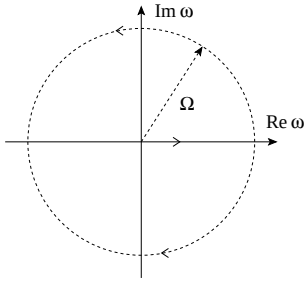


FIG. 7: Two different ways to close the integration contour on the complex frequency plane.

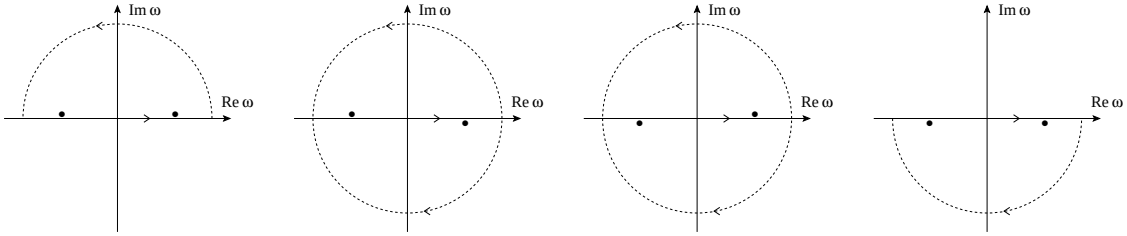


FIG. 8: The poles of the four kinds of Green's function of eqs. (B12).

We may close the integration contour over either the upper or the lower half circle as shown in Fig. 7. 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

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

defining the advanced (D^a), the Feynman (D_F) and the retarded (D^a) Green's functions.

Example: Consider a damped harmonic oscillator, driven by an external source. The equation of motion is

$$m\ddot{x} = -m\omega_0^2 x - k\dot{x} - j \tag{B13}$$

and the source is a Gaussian, localised at $t = 0$,

$$j(t) = j_0\frac{\xi}{\sqrt{2\pi}}e^{-\frac{\xi^2}{2}t^2}. \tag{B14}$$

and normalized to have $\int dtj(t) = j_0$. What is the trajectory $x(t)$, corresponding to the initial conditions $x(-\infty) = \dot{x}(-\infty) = 0$?

The Fourier transform of the equation of motion,

$$m\int dte^{i\omega t}\ddot{x}(t) = -m\omega_0^2\int dte^{i\omega t}x(t) - k\int dte^{i\omega t}\dot{x}(t) - \int dte^{i\omega t}j(t), \tag{B15}$$

can be written in the form

$$(\omega^2 - \omega_0^2 + i\nu\omega_0)\tilde{x}(\omega) = \frac{1}{m}\tilde{j}(\omega), \tag{B16}$$

where $\nu = k/m$ and

$$\tilde{f}(\omega) = \int dte^{i\omega t}f(t). \tag{B17}$$

Some partial integrations were performed in the time integrals and the boundary term can be neglected according to the Riemann-Lesbegue lemma owing to its fast oscillation. Eq. (B16) yields the Green's function

$$D(\omega) = \frac{1}{m[(\omega + i\epsilon)^2 - \omega_0^2 + i\nu\omega]} \to \frac{1}{m(\omega^2 - \omega_0^2 + i\nu\omega)}. \tag{B18}$$

Note that ϵ can be omitted since the friction force renders Green's function,

$$D(t) = \lim_{\Omega\to\infty}\int_{-\Omega}^{\Omega}\frac{d\omega}{2\pi}\frac{e^{-i\omega t}}{m(\omega^2 - \omega^2 + i\nu\omega)} \tag{B19}$$

retarded. The poles

$$\omega_\pm = -i\frac{\nu}{2} \pm \Omega \tag{B20}$$

with $\Omega = \sqrt{\omega_0^2 - \frac{\nu^2}{4}}$ allows us to find easily the integral,

$$\begin{aligned} D(t) &= \frac{1}{m}\lim_{\Omega\to\infty}\int_{-\Omega}^{\Omega}\frac{d\omega}{2\pi}\frac{e^{-i\omega t}}{(\omega - \omega_+)(\omega - \omega_-)} \\ &= i\Theta(t)\frac{e^{-i\omega_- t} - e^{-i\omega_+ t}}{2m\Omega} \\ &= -\Theta(t)e^{-\frac{\nu}{2}t}\frac{\sin\Omega t}{m\Omega}. \end{aligned} \tag{B21}$$

Hence the trajectory is

$$\begin{aligned} x(t) &= \int dtD(t - t')j(t') \\ &= ij_0\frac{\xi}{\sqrt{2\pi}}\int dt'\frac{e^{-i\omega_-(t-t')} - e^{-i\omega_+(t-t')}}{2m\Omega}e^{-\frac{\xi^2}{2}t'^2}. \end{aligned} \tag{B22}$$

The Gaussian integral with $a > 0$,

$$\int dt e^{-\frac{a}{2}t^2+bt} = \sqrt{\frac{2\pi}{a}} e^{\frac{b^2}{2a}}, \tag{B23}$$

yields

$$\begin{aligned} x(t) &= i\frac{j_0}{2m\Omega}(e^{-i\omega_- t-\frac{\omega_-^2}{2\xi^2}} - e^{-i\omega_+ t-\frac{\omega_+^2}{2\xi^2}}) \\ &= -\frac{j_0}{m\Omega} e^{-\frac{\nu}{2}t} \mathrm{Im} e^{i\Omega t-\frac{\omega_-^2}{2\xi^2}} \end{aligned} \tag{B24}$$

in the underdamped case, $2\omega_0 > \nu$ and

$$x(t) = \frac{\sqrt{2\pi} j_0}{2m\xi|\Omega|} e^{-\frac{\nu}{2}t} \left[e^{-|\Omega|t+\frac{(\frac{\nu}{2}+|\Omega|)^2}{2\xi^2}} - e^{|\Omega|t+\frac{(\frac{\nu}{2}-|\Omega|)^2}{2\xi^2}} \right] \tag{B25}$$

for the overdamped oscillator.

2. Electromagnetic field

The formal Green's function of the wave equation (11),

$$D(x-x') = \int \frac{d^4q}{(2\pi)^4} e^{-iq(x-x')} \tilde{D}(q), \tag{B26}$$

is given by

$$\tilde{D}(q) = \begin{cases} -\frac{1}{q^2} & q^2 \neq 0, \\ ? & q^2 = 0, \end{cases} \tag{B27}$$

$q^2 = q^{02} - \boldsymbol{q}^2$. 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,

$$\begin{aligned} D^r(x) &= -\int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{k}\boldsymbol{x}} \int \frac{dk_0}{2\pi} \frac{e^{-ick_0 t}}{(k_0 + i\epsilon - |\boldsymbol{k}|)(k_0 + i\epsilon + |\boldsymbol{k}|)} \\ &= i\Theta(t) \int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{k}\boldsymbol{x}} \left(\frac{e^{-ickt}}{2k} - \frac{e^{ickt}}{2k} \right) \\ &= \frac{i\Theta(t)}{(2\pi)^3} \int dk k^2 d\phi d(\cos\theta) e^{ikr\cos\theta} \frac{e^{-ickt} - e^{ickt}}{2k} \\ &= \frac{i\Theta(t)}{(2\pi)^2} \int dk k^2 \frac{e^{ikr} - e^{-ikr}}{ikr} \frac{e^{-ickt} - e^{ickt}}{2k} \\ &= \frac{\Theta(t)}{2(2\pi)^2 r} \int_0^\infty dk (e^{ikr} - e^{-ikr})(e^{-ickt} - e^{ickt}) \\ &= \frac{\Theta(t)}{8\pi r} \int_{-\infty}^\infty \frac{dk}{2\pi} (e^{ik(r-ct)} + e^{ik(-r+ct)} - e^{-ik(r+ct)} - e^{ik(r+ct)}) \\ &= \frac{\Theta(t)}{4\pi r} [\delta(-r+ct) - \delta(r+ct)] \\ &= \frac{\delta(ct-r)}{4\pi r}. \end{aligned} \tag{B28}$$

The advanced Green's function is given by

$$\begin{aligned} D^a(x) &= -\int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{kx}} \int \frac{dk_0}{2\pi} \frac{e^{-ick_0t}}{(k_0 - i\epsilon - |\boldsymbol{k}|)(k_0 - i\epsilon + |\boldsymbol{k}|)} \\ &= i\Theta(-t) \int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{kx}} \left(\frac{e^{ickt}}{2k} - \frac{e^{-ickt}}{2k} \right) \\ &= \Theta(-t) \frac{\delta(r+ct) - \delta(-r+ct)}{4\pi r} \\ &= \frac{\delta(ct+r)}{4\pi r}. \end{aligned} \tag{B29}$$

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

$$\begin{aligned} \overset{r}{D^a}(x) &= \Theta(\pm t) \frac{\delta(ct \mp r)}{4\pi r} \\ &= \Theta(\pm t) \frac{\delta(ct+r) + \delta(ct-r)}{4\pi r} \\ &= \Theta(\pm t) \frac{\delta(c^2t^2 - r^2)}{2\pi} \\ &= \Theta(\pm x^0) \frac{\delta(x^2)}{2\pi}. \end{aligned} \tag{B30}$$

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

$$\overset{n}{D^f} = \frac{1}{2}(D^r \pm D^a) \tag{B31}$$

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

$$\overset{r}{D^a}(x,y) = 2D^n(x,y)\Theta(\pm(x^0 - y^0)) \tag{B32}$$

where the near field Green's function is

$$D^n(x) = \frac{\delta(x^2)}{4\pi} \tag{B33}$$

according to Eq. (B30). The Fourier representation of the homogeneous far Green's function can be obtained by considering the difference of the second lines in Eqs. (B28) and (B29),

$$\begin{aligned} D^f(x) &= \frac{1}{4\pi}\delta(x^2)\epsilon(x^0) \\ &= -\frac{i}{2} \int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{kx}} \left(\frac{e^{ickt}}{2k} - \frac{e^{-ickt}}{2k} \right) \\ &= \frac{i}{2} \int \frac{d^4k}{(2\pi)^3} e^{-ikx} \frac{\delta(k_0 - |\boldsymbol{k}|) - \delta(k_0 + |\boldsymbol{k}|)}{2|\boldsymbol{k}|} \\ &= \frac{i}{2} \int \frac{d^4k}{(2\pi)^3} e^{ikx} \delta(k^2)\epsilon(k_0) \end{aligned} \tag{B34}$$

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

$$\begin{aligned}\partial_{x^0} D^f(x)_{x^0=0} &= \frac{1}{2}\int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{k}\boldsymbol{x}} k_0 \frac{\delta(k_0 - |\boldsymbol{k}|) - \delta(k_0 + |\boldsymbol{k}|)}{2|\boldsymbol{k}|} \\ &= \frac{1}{2}\int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{k}\boldsymbol{x}} \frac{1}{2}[\delta(k_0 - |\boldsymbol{k}|) + \delta(k_0 + |\boldsymbol{k}|)] \\ &= \frac{1}{2}\delta(\boldsymbol{x}) \end{aligned} \tag{B35}$$

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: Information in physics

The concept of information is obviously important in communication but its relevance in physics has been recognized gradually only. The first, mathematically well defined use of information is due Claude Shannon, an electric engineer, who has characterized the usefulness of data compression 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 E. T. 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.

So far everything is simple, however complications arise when we do not possess all information needed for the algorithms. If we have all information about a classical system then the deterministic

laws of classical physics preserve this state and no information theoretical approach is needed. But facing a complicated systems we may have a subjective limitation, imposed by our finite capabilities. We then rely on the probability theory to transform our initial partial information into other, similarly partial informations. While the very reason of working with probability is our subjective limitation the way we proceed is objective in the sense that it is consistent, i.e. any observer, finding the same observations agree with us and come to the same (probabilistic) conclusion.

The missing classical information exists "out there", simply we do not want or can not acquire it. The rules of quantum mechanics are different, the lesson of Heisenberg's uncertainty principle being that we can never possess all information about a system. Quantum mechanics consists of the rules of systematic and optimized use of partial informations, expressed in terms of probabilities. Hence there is a fundamental difference between the probabilities, appearing in classical and quantum physics, namely the former are due to our (as data receiver) limitations and the latter is an unavoidable feature of Nature.

Whatever is the reason of missing information, we use probabilities from now and face the problem of acquiring and handling probabilities instead of fully specified facts. But how to measure, i.e. determine experimentally a probability? The measurement of a physical quantity, performed in a limited space-time region, places the value of the quantity in question within a well defined interval with length, determined by macroscopic considerations. But the measurement of a probability consists of the registration of a relative frequency and the law of large numbers asserts that more events we use in this process less is the probability of a given, fixed deviation between the observed relative frequency and the probability. There are two lessons of this theorem: The probability is defined in a circular manner and there is no way to measure it in our life with a finite error bar.

One can not postpone anymore the question concerning the very essence of the probability: Does probability belong to Nature or is it a concept, created by us, reflecting our way of reasoning? It is clear that any attempt to follow this line of thought leads to neurology and the functioning of our neurons on the molecular level. We on a pragmatic level and use the probability as a way to encode partial informations, independently of the philosophical background.

1. Shannon information

The appearance of probability in our arguments indicates a loss of information. How to quantify the latter? Any answer to this question comes up with a number which is independent of the actual

spectrum of the probability variable and depends on the probability distribution only. Thus seek the missing information, $I[p]$, defined for probability distributions.

Let us consider 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,

$$I_{nm} = I_n + I_m. \tag{D1}$$

The simple solution,

$$I = \ln \Omega, \tag{D2}$$

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

$$\langle I_g \rangle = \sum_{j=1}^{n} p_j \ln \ell_j \tag{D3}$$

according to Eq. (D2), leading to

$$I[p] = I_t - \langle I_g \rangle = -\sum_{j=1}^{\ell} p_j \ln p_j. \tag{D4}$$

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 (D2),

$$I[p] = \ln \Omega[p], \tag{D5}$$

where the number of the allowed series,

$$\Omega[p] = \frac{N!}{\prod_j (Np_j)!}. \tag{D6}$$

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

$$\begin{aligned} I[p] &= N \ln N - N - N \sum_j p_j \ln N p_j + N \sum_j p_j \\ &= -N \sum_j p_j \ln p_j \end{aligned} \tag{D7}$$

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

$$S[p] = \frac{I[p]}{N} = -\sum_j p_j \ln p_j = -\langle \ln p \rangle, \tag{D8}$$

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

$$2^{N_Q} = \Omega[p] = e^{-N \sum_j p_j \ln p_j} \tag{D9}$$

and

$$N_q \ln 2 = \frac{\text{missing information}}{\text{symbol}}, \tag{D10}$$

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

2. 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 $f_k(x)$, $k=1,\ldots,m$,

$$\frac{1}{N}\sum_j \boldsymbol{f}(x(t_j)) = \boldsymbol{F}. \tag{D11}$$

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

$$\sum_j p_j \boldsymbol{f}(x_j) = \boldsymbol{F}. \tag{D12}$$

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

$$S_F = -\sum_j p_j \ln p_j + (1-\lambda_0)(\sum_j p_j - 1) + \boldsymbol{\lambda}(\boldsymbol{F} - \sum_j p_j \boldsymbol{f}(x_j)) \tag{D13}$$

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

$$0 = -\ln p_j - 1 - \lambda_0 + 1 - \boldsymbol{\lambda}\boldsymbol{f}(x_j), \tag{D14}$$

fixes the probability distribution,

$$p_j = e^{-\lambda_0 - \boldsymbol{\lambda}\boldsymbol{f}(x_j)}, \tag{D15}$$

and the maximization in λ_0 yields the partition function,

$$\frac{\partial}{\partial\lambda_0} \;:\; 1 = e^{-\lambda_0} Z(\boldsymbol{\lambda}), \quad Z(\boldsymbol{\lambda}) = \sum_j e^{-\boldsymbol{\lambda}\boldsymbol{f}(x_j)} = e^{\lambda_0}. \tag{D16}$$

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

$$\frac{\partial}{\partial\boldsymbol{\lambda}} \;:\; \boldsymbol{F} = e^{-\lambda_0}\sum_j \boldsymbol{f}(x_j) e^{-\boldsymbol{\lambda}\boldsymbol{f}(x_j)} = \frac{1}{Z(\boldsymbol{\lambda})}\sum_j \boldsymbol{f}(x_j) e^{-\boldsymbol{\lambda}\boldsymbol{f}(x_j)} = -\frac{\partial \ln Z(\boldsymbol{\lambda})}{\partial\boldsymbol{\lambda}}. \tag{D17}$$

The value of the maximal entropy is

$$\begin{aligned} S_{max} &= -\sum_j p_j \ln p_j \\ &= \sum_j e^{-\lambda_0 - \boldsymbol{\lambda}\boldsymbol{f}(x_j)}[\lambda_0 + \boldsymbol{\lambda}\boldsymbol{f}(x_j)] \\ &= \lambda_0 + \boldsymbol{\lambda}\boldsymbol{F}. \end{aligned} \tag{D18}$$

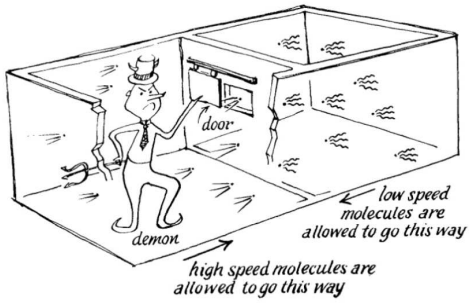


FIG. 9: Maxwell's demon after W. F. Angrist and L. G. Hepler, *Order and Chaos* (Basic Books, New York, 1967)

3. 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 informations. 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

$$\sum_j p_j (s_j + \ln p_j) \geq 0 \tag{D19}$$

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

$$\sum_j e^{-S_j} \leq 1. \tag{D20}$$

In particular, a demon, working in a reversible manner and producing the entropy $\Delta S = \ln 2$ remains in agreement with thermodynamics. The inequality (D19) 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

The description of open quantum systems requires the generalization some fundamental ideas of quantum mechanics, developped for closed systems only. The density matrix representation of the states of an open quantum system is introduced here.

1. Uncertainty about the quantum state

The usual introduction to quantum mechanics addresses a part of the subject only: There is a detailed discussion of how to calculate expectation values, assuming that the system is or has been in a given state. The inverse problem, the determination of the quantum state by the help of measurement, the quantum inference, is usually ignored. Let us suppose that the repeated measurements of the observable A on a set of identically prepared systems we can infer a probability distribution, p_n, to find the system in the states, $|\psi_n\rangle$. This distribution reflects our limited way of handling the informations and we are sure in the meantime that the system is in some state, characterized by a vector of the Hilbert space. This probability is classical in the sense that it is

due to the loss of otherwise existing information. The expectation value of A is therefore

$$\langle A\rangle = \sum_n p_n \langle\psi_n|A|\psi_n\rangle = \mathrm{Tr}[\rho A] \tag{E1}$$

where the density matrix,

$$\rho = \sum_n |\psi_n\rangle p_n \langle\psi_n|, \tag{E2}$$

is the generalized representation of the quantum state.

The probability of finding the system which is in the state $|\psi\rangle$ in the state $|\phi\rangle$ is

$$P(\psi \to \phi) = |\langle\phi|\psi\rangle|^2 \tag{E3}$$

according to the Born rule. This probability can be written as the expectation value of the projector, $P_\phi = |\phi\rangle\langle\phi|$ in the state $|\psi\rangle$,

$$P(\psi \to \phi) = \langle\psi|\phi\rangle\langle\phi|\psi\rangle] = \mathrm{Tr}[P_\phi|\psi\rangle\langle\psi|], \tag{E4}$$

showing that p_n in (E2) can be identified with the probability of finding the system in the state $|\phi_n\rangle$.

Note the additivity in the probability, p_n, and the absence of the interference between the states $|\psi_n\rangle$ in (E1). In contrast, the average of A in the pure state, $|\psi\rangle = \sum_n \sqrt{p_n}|\psi_n\rangle$,

$$\langle\psi|A|\psi\rangle = \sum_{mn} \sqrt{p_m p_n}\langle\psi_m|A|\psi_n\rangle, \tag{E5}$$

contains the interference terms which destroy the additity in p_n. Decoherence, the destruction of the coherence among macroscopically different states, generates classical probabilities for macroscopically different quantum states.

2. Properties

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

$$\rho = \sum_n |\psi_n\rangle p_n \langle\psi_n|, \tag{E6}$$

$\{|\psi_n\rangle\}$ 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

$$\mathrm{Tr}A\rho = \sum_n p_n \langle\psi_n|A|\psi_n\rangle. \tag{E7}$$

5. The inequality

$$\mathrm{Tr}p^2 = \sum_n p_n^2 \leq \sum_n p_n = \mathrm{Tr}\rho \tag{E8}$$

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

$$\rho = \frac{1}{2}(\mathbb{1} + \boldsymbol{p}\boldsymbol{\sigma}) \tag{E9}$$

where the Pauli-matrices are

$$\boldsymbol{\sigma} = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right). \tag{E10}$$

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

$$\langle\boldsymbol{\sigma}\rangle = \mathrm{tr}\rho\boldsymbol{\sigma} = \boldsymbol{p}. \tag{E11}$$

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

$$p(E) = \frac{1}{Z} e^{-\frac{E}{k_B T}}, \quad Z = \sum_E e^{-\frac{E}{k_B T}}. \tag{E12}$$

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

$$\rho = \frac{1}{Z} e^{-\frac{H}{k_B T}}, \quad Z = \mathrm{Tr} e^{-\frac{H}{k_B T}}. \tag{E13}$$

3. Unobserved environment

There is a simple, natural way modelling the missing information about the quantum state, namely that the missing information belongs to an unobserved environment.

We begin by recalling the representation of composite quantum systems. Let us consider two systems, represented by the linear spaces, $\mathcal{H}_j$, $j = 1, 2$. The states of the composite system can be constructed by the help of the pairs $(|\psi_1\rangle, |\psi_2\rangle)$, denoted by $|\psi_1\rangle \otimes |\psi_2\rangle$, $|\psi_j\rangle \in \mathcal{H}_j$. These pairs make up a linear space, called the direct product, $\mathcal{H}_{1\otimes 2} = \mathcal{H}_1 \otimes \mathcal{H}_2$, with the following structure:

1. Multiplication:

$$(c|\psi_1\rangle) \otimes |\psi_2\rangle = |\psi_1\rangle \otimes (c|\psi_2\rangle) = c(|\psi_1\rangle \otimes |\psi_2\rangle). \tag{E14}$$

2. Addition: $\mathcal{H}_1 \otimes \mathcal{H}_2$ is closed with respect to addition within $\mathcal{H}_1$, $\mathcal{H}_2$ and $\mathcal{H}_1 \otimes \mathcal{H}_2$:

$$\begin{aligned} &|\psi_1\rangle \otimes |\psi_2\rangle, \quad |\psi_1'\rangle \otimes |\psi_2'\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \quad \rightarrow \quad |\psi_1\rangle \otimes |\psi_2\rangle + |\psi_1'\rangle \otimes |\psi_2'\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \\ &|\psi_1\rangle, |\psi_1'\rangle \in \mathcal{H}_1, \quad \rightarrow \quad |\psi_1\rangle \otimes |\psi_2\rangle + |\psi_1'\rangle \otimes |\psi_2'\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \end{aligned} \tag{E15}$$

3. Scalar product:

$$(\langle\psi_1| \otimes \langle\psi_2|)(|\psi_1'\rangle \otimes |\psi_2'\rangle) = \langle\psi_1|\psi_1'\rangle\langle\psi_2|\psi_2'\rangle. \tag{E16}$$

4. A pair of operators, $A_j : \mathcal{H}_j \rightarrow \mathcal{H}_j$ defines $A_1 \otimes A_2 : \mathcal{H}_{1\otimes 2} \rightarrow \mathcal{H}_{1\otimes 2}$, as

$$\langle\psi_1| \otimes \langle\psi_2|A_1 \otimes A_2|\psi_1'\rangle \otimes |\psi_2'\rangle = \langle\psi_1|A_1|\psi_1'\rangle\langle\psi_2|A_2|\psi_2'\rangle. \tag{E17}$$

These properties suggest to represent the direct product of vectors by multiplying their components, $\langle j_1, j_2|\psi_1\rangle \otimes |\psi_2\rangle = \langle j_1|\psi_1\rangle\langle j_2|\psi_2\rangle$, and $(\psi_1 \otimes \psi_2)(x_1, x_2) = \psi_1(x_1)\psi_2(x_2)$ with $\psi(x) = \langle x|\psi\rangle$, in terms of the bra-kets and the wave functions, respectively. If the set $\{|n_j\rangle\}$ is a basis for $\mathcal{H}_j$ then $\{|m_1\rangle \otimes |n_2\rangle|$ is a basis for $\mathcal{H}_{1\otimes 2}$ and $\dim \mathcal{H}_{1\otimes 2} = \dim \mathcal{H}_1 \dim \mathcal{H}_2$.

Let us now return to the discussion of the emergence of mixed state and assume that the Hilbert space of states of the full, closed system is the direct product, $\mathcal{H}_{se} = \mathcal{H}_s \otimes \mathcal{H}_e$, of the system and

the environment Hilbert spaces, $\mathcal{H}_s$ and $\mathcal{H}_e$, respectively. We introduce the bases $|\phi_m\rangle \in \mathcal{H}_s$ and $|\chi_n\rangle \in \mathcal{H}_e$ and write a state of the complete system as a linear superposition,

$$|\psi\rangle = \sum_{m,n} c_{m,n}|m,n\rangle. \tag{E18}$$

where $|m,n\rangle = |\phi_m\rangle \otimes |\chi_n\rangle$. A state, $|\psi\rangle = |\phi\rangle| \otimes |\chi\rangle$, consisting of a single contribution is called factorisable and state which is the sum of more than one factorisable states is called entangled.

The properties of a sub-system are well defined as long as the whose system is in a factorisable state. An observable A_s of our system is represented by the operator $A = A_s \otimes \mathbb{1}$ and its expectation values in a factorisable state, $|\psi\rangle = |\phi\rangle| \otimes |\chi\rangle$,

$$\langle\psi|A|\psi\rangle = \langle\phi|A_s|\phi\rangle, \tag{E19}$$

is indeed determined by the unique state $|\phi\rangle$ of the sub-system. However the expectation value of system observable in an entangled state (E18),

$$\langle A\rangle = \sum_{m,n,m'} c_{m,n}c^*_{m',n}\langle\phi_{m'}|A_s|\phi_m\rangle, \tag{E20}$$

is made up by the matrix elements of A_s among different system states, $|\phi_m\rangle$. This expectation value can be reproduced in the form $\mathrm{Tr}\rho_r A^{(1)}$ in terms of the reduced density matrix,

$$\rho_r = \sum_{m,n,m'} |\phi_m\rangle c_{m,n}c^*_{m',n}\langle\phi_{m'}| = \mathrm{Tr}_e\rho, \tag{E21}$$

where Tr_e denotes the trace over the environment space.

It is important to realize that the system expectation values *can not* be represented by a pure state in case of system-environment entanglement. In fact, let us suppose that the contrary is true, the complete system state, (E18) is entangled and the system expectation values can be calculated by using the system state $|\phi_{obs}\rangle$. We use this receipt for the calculation of the probability of finding the system in the state $|\phi_{obs}\rangle$,

$$\begin{aligned} p_{\phi_{obs}} &= \sum_{m,m',n,n'} c^*_{m',n'}c_{m,n}\langle m',n'|(|\phi_{obs}\rangle\langle\phi_{obs}| \otimes \mathbb{1})|m,n\rangle \\ &= \sum_{m,m',n} c^*_{m',n}c_{m,n}\langle m'|\phi\rangle\langle\phi|m\rangle. \end{aligned} \tag{E22}$$

One the one hand, the normalization $\sum_{m,n}|c_{m,n}|^2 = 1$ and the bound $|\langle m|\phi_{obs}\rangle| \leq 1$ gives $p_\phi < 1$ for entangled states which contain at least two non-vanishing contributions in (E18). On the other hand, we must have $p_\phi = 1$.

The lesson is that no unique property, characterized the eigenvalues of A_s, can be assigned to the system without some reference to the environment for entangled states, the environment contains some information, missing in the system. The interactions between the two sub-systems generate entanglement except of the irrelevant special case where the interaction Hamiltonian is diagonal in the given basis. But entanglement is a more general concept than interactions because the latter is defined by the interaction energy and former is a property of the state of the complete system, without any reference to the system-environment interactions.

Both the loss of classical informations and the entanglement are represented by the same mathematical device, a mixed state. Therefore one tends to consider entanglement as the physical origin of mixed states and the modelization of lost classical informations at the more fundamental quantum level.

4. Relative states

The correlation between the system and its environment can better be seen by introducing the relative states. For any pure complete system state $|\psi\rangle$ the relative state of an environment state vector, $|\chi\rangle$, is defined by

$$|R(\chi)\rangle = N \sum_m |\phi_m\rangle\langle\phi_m, \chi|\psi\rangle, \tag{E23}$$

where the notation $|\phi_m, \chi\rangle = |\phi_m\rangle \otimes |\chi\rangle$ is introduced and $N = 1/\sqrt{p}$ denotes the normalization, defined by the marginal probability distribution,

$$\begin{aligned} p(\chi) &= \sum_m |\langle\phi_m, \chi|\psi\rangle|^2 \\ &= \langle\psi|(\mathbb{1} \otimes |\chi\rangle\langle\chi|)|\psi\rangle, \end{aligned} \tag{E24}$$

of the environment states in $|\psi\rangle$. One can prove that the relative state and the marginal probabilities are independent of the choice of the system basis, $|\phi_m\rangle$.

Let us consider a system observable which is diagonal in our basis, $A_s = \sum_m |\phi_m\rangle\lambda_m\langle\phi_m|$. Its expectation value in a relative state, assuming that the environment is in the pure state $|\chi\rangle$,

$$\langle R(\chi)|A_s|R(\chi)\rangle = \frac{1}{p(\chi)} \sum_m \langle\psi|\phi_m, \chi\rangle\langle\phi_m, \chi|A_s \otimes \mathbb{1}|\phi_m, \chi\rangle\langle\phi_m, \chi|\psi\rangle, \tag{E25}$$

can be written as

$$\langle R(\chi)|A_s|R(\chi)\rangle = \sum_m \lambda_m \frac{\langle\phi_m, \chi|\psi\rangle|^2}{p(\chi)}. \tag{E26}$$

Since the factor $p(\phi_m|\chi) = \langle\phi_m, \chi|\psi\rangle|^2/p(\chi)$ is just the conditional probability of finding the system state $|\phi_m\rangle$, assuming that the environment is in the state $|\chi\rangle$, we have

$$\langle R(\chi)|A_s|R(\chi)\rangle = \sum_m \lambda_m p(\phi_m|\chi), \tag{E27}$$

indicating that the knowledge of the environment state translates itself into the relative system states, as far as the system observables are concerned. The pure complete system state can be written as

$$|\psi\rangle = \sum_{m,n} |\phi_m, \chi_n\rangle\langle\phi_m, \chi_n|\psi\rangle = \sum_n \sqrt{p(\chi_n)}|R(\chi_n)\rangle \otimes |\chi_n\rangle \tag{E28}$$

We now return to the discussion of the density matrix and write the expectation value of the system observable, A_s, in the pure complete system state, $|\psi\rangle$, as

$$\begin{aligned}\langle\psi|A_s|\psi\rangle &= \sum_{n,n'} \sqrt{p(\chi_n)p(\chi_{n'})}\langle R(\chi_{n'})| \otimes \langle\chi_{n'}|A_s \otimes \mathbb{1}|R(\chi_n)\rangle \otimes |\chi_n\rangle \\ &= \sum_n p(\chi_n)\langle R(\chi_n)|A_s|R(\chi_n)\rangle.\end{aligned} \tag{E29}$$

In other words, the reduced density matrix is

$$\rho = \sum_n |R(\chi_n)\rangle p(\chi_n)\langle R(\chi_n)|. \tag{E30}$$

The lesson is that entanglement arises if different environment states can condition linearly independent system states in the given pure complete system state.

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 (D19) 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 (D19) 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 (D20).