THE PHYSICS OF PROGRAMS

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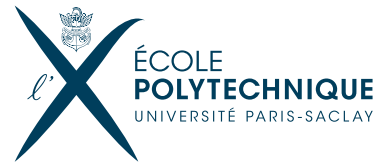


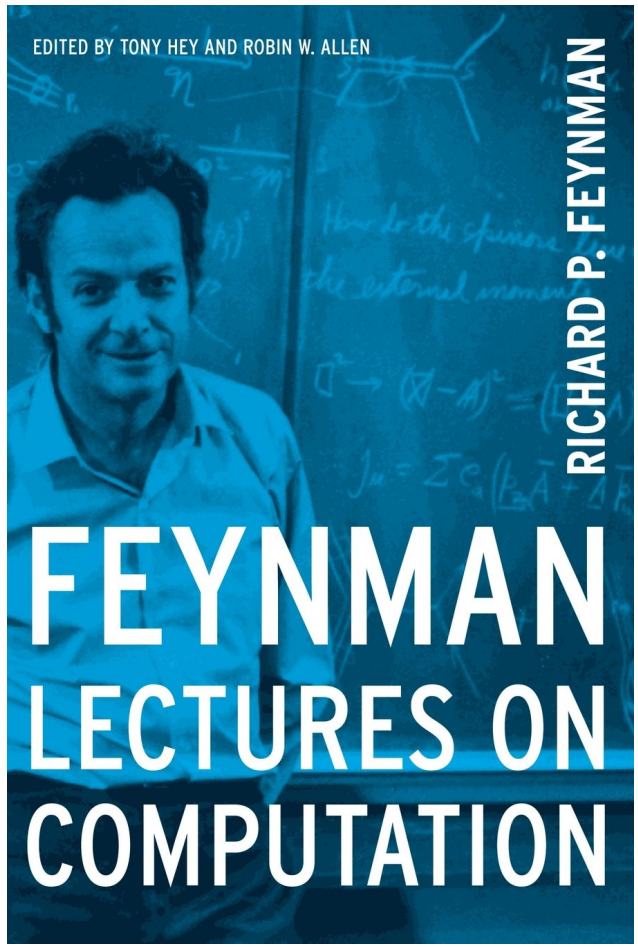
Séminaire Cosynus

February 23, 2018

The Universe is executing a program.

Blame it on Feynman

I had some intuitions about analogies between physic and semantics of programs and then I read [Fey96]:



our aim is to exhibit some Hamiltonian for a system which could serve as a computer.

THERMODYNAMICS

Information

Consider a set with n equiprobable elements.

The **information** brought by an element is

$$\log_2(n)$$

It can namely be identified by a string of $\log_2(n)$ bits.

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Writing $p = \frac{1}{n}$ for the probability, the information is thus

$$I(p) \quad = \quad \log_2(n) \quad = \quad \log_2\left(\frac{1}{p}\right) \quad = \quad -\log_2(p)$$

Information

If each element x_i has probability p_i, the mean information is called the **entropy**:

$$S = \sum_i P(x_i) I(x_i) = -\sum_i p_i \log_2(p_i)$$

Information

A function $I(p)$ for information should be

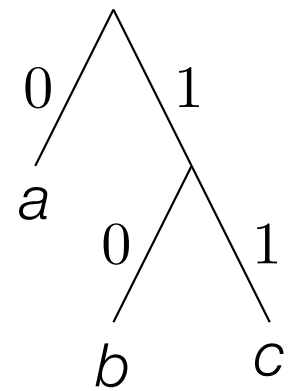
1. anti-monotonic: $p_1 \leq p_2$ implies $I(p_1) \geq I(p_2)$
2. positive: $I(p) \geq 0$
3. $I(1) = 0$
4. $I(p_1 p_2) = I(p_1) + I(p_2)$

The entropy is the only function satisfying this.

For instance, consider $\{a, b, c\}$ with

$$p(a) = \frac{1}{2} \qquad p(b) = \frac{1}{4} \qquad p(c) = \frac{1}{4}$$

These can be encoded as



and

$$\begin{aligned} S &= -\frac{1}{2}\log_2\left(\frac{1}{2}\right) - \frac{1}{4}\log_2\left(\frac{1}{4}\right) - \frac{1}{4}\log_2\left(\frac{1}{4}\right) \\ &= \frac{1}{2}\log_2(2) + \frac{1}{2}\log_2(4) \\ &= 1.5 \end{aligned}$$

Gas

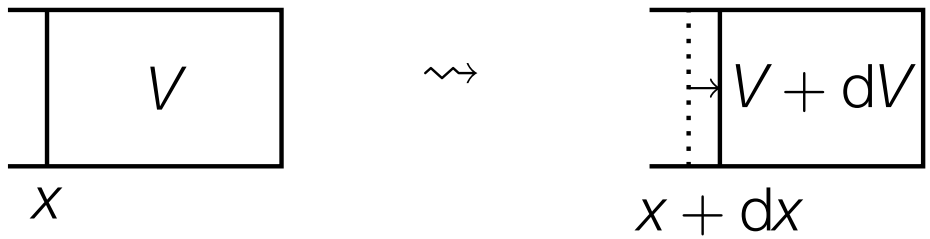
Given a gas, the **pressure** P such that the resulting force is

$$F = PA$$

where A is the surface.

Compression

Given a piston



the work done on the gas is

$$\mathrm{d}W = F\,\mathrm{d}x$$

or equivalently

$$\mathrm{d}W = PA\,\mathrm{d}x = P\,\mathrm{d}V$$

Compression

We know that

$$PV = NkT$$

where

- N: number of particles
- $k = 1.38 \times 10^{-23}\ \mathrm{J\,K^{-1}}$
- T: temperature
- kT: (proportional to) the mean kinetic energy of particles

Compression

The work is thus

$$\mathrm{d}W = \int_{V_1}^{V_2} NkT\frac{\mathrm{d}V}{V}$$

Compression

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$$\mathrm{d}W = \int_{V_1}^{V_2} NkT \frac{\mathrm{d}V}{V}$$

If the compression is *isothermal* (no change in T):

$$W = NkT \log \frac{V_2}{V_1}$$

(this work is energy given to the environment!)

Firs law of thermodynamics

The **internal energy** U satisfies

$$\mathrm{d}U \quad = \quad \delta Q + \mathrm{d}W$$

where

- δQ is the heat brought to the system
- $\mathrm{d}W$ is the work done on the system

In our compression, $\mathrm{d}U = 0$ so that

$$Q \quad = \quad -W$$

Second law of thermodynamics

There is a quantity called **entropy** with

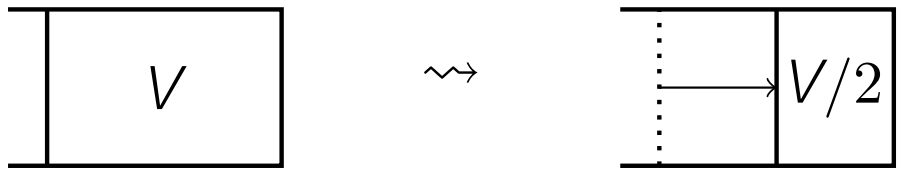
$$\mathrm{d}S \quad \geq \quad \frac{\delta Q}{T}$$

with equality for a **reversible** process:

- gas is at equilibrium,
- same temperature as surroundings,
- etc.

Compression

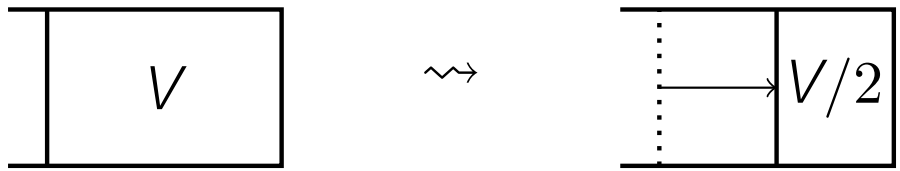
Suppose that we half the volume, with same temperature



We have

$$\begin{aligned} \Delta S &= \frac{\Delta Q}{T} \\ &= \frac{NkT \log\left(\frac{V}{2V}\right)}{T} \\ &= -Nk \log(2) \end{aligned}$$

Compression



In particular for $N = 1$ particle, halving the volume means

$$\Delta S \quad = \quad -k \log(2)$$

We have gained one bit of information! (up to a multiplicative constant)

Entropy

Boltzmann developed a statistical definition of **entropy**:

$$S = -k \sum_i p_i \ln(p_i)$$

where

- k is the Boltzmann constant,
- i ranges over possible microstates giving rise to the macrostate.

In other words, S says how precisely we know what's in the box.

REVERSIBLE COMPUTING

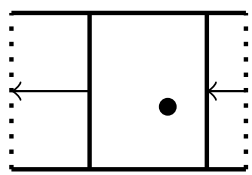
Information in a tape

The information in a finite boolean tape

$\cdots$	0	1	1	$?$	$?$	0	$?$	1	0	$?$	$\cdots$

is the free energy required to reset the tape to 0 [Lan61]:

- if we know it is a 0, there is nothing to do
- if we know it is a 1 then it takes no energy to put it to 0:



- if we don't know what it is it takes energy to put it to 0:

$$W \quad = \quad kT\log(2)$$

Reversible computations

A computation is **reversible** if no data if ever erased.

For those there is no lower limit on the consumed energy!

[1] excepting in billiard ball, but here we are sensitive to fluctuations…

Reversible computations

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This is wonderful but:

- bit erasure accounts for $1/10000$-th of the consumed energy in a CPU today,
- they have to be run at infinitesimal speed, otherwise we loose energy: if we want the computer to have r times more chance to run forward than backwards then each step requires[1]

$$kT\log(r)$$

[1] excepting in billiard ball, but here we are sensitive to fluctuations…

Reversible boolean circuits

A boolean circuit is **reversible** if no information is lost.

Otherwise said, I can recover the inputs from the outputs.

Otherwise said, it computes an injective boolean function.

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Example

- NOT is reversible
- AND, OR, XOR are not reversible

Reversible gates

The gate

$$\mathsf{NOT} \quad : \quad \mathbb{B} \to \mathbb{B}$$

is reversible:

i_0	o_0
0	1
1	0

Reversible gates

The **controlled not** gate

$$\text{CNOT} \quad : \quad \mathbb{B}^2 \to \mathbb{B}^2$$

is reversible:

i_0	i_1	o_0	o_1
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

Reversible gates

The **controlled controlled not** (or Toffoli) gate

$$\text{CCNOT} \quad : \quad \mathbb{B}^3 \to \mathbb{B}^3$$

is reversible: last bit is inverted in both other are true.

i_0	i_1	i_2	o_0	o_1	o_2
0	0	0	0	0	0
0	0	1	0	0	1
0	1	0	0	1	0
0	1	1	0	1	1
1	0	0	1	0	0
1	0	1	1	0	1
1	1	0	1	1	1
1	1	1	1	1	0

Reversible gates

The **controlled swap** (or Fredkin) gate

$$\text{CSWAP} \quad : \quad \mathbb{B}^3 \to \mathbb{B}^3$$

is reversible: last two bits are exchanged if first is true.

i_0	i_1	i_2	o_0	o_1	o_2
0	0	0	0	0	0
0	0	1	0	0	1
0	1	0	0	1	0
0	1	1	0	1	1
1	0	0	1	0	0
1	0	1	1	1	0
1	1	0	1	0	1
1	1	1	1	1	1

Reversible gates

The **swap** gate

$$\mathrm{SWAP} \quad : \quad \mathbb{B} \quad \to \quad \mathbb{B}^2$$

is reversible:

i_0	i_1	o_0	o_1
0	0	0	0
0	1	1	0
1	0	0	1
1	1	1	1

Reversible gates

Perhaps more surprisingly, the **duplicator**

$$\mathrm{DUP} \quad : \quad \mathbb{B} \quad \to \quad \mathbb{B}^2$$

is also reversible:

i_0	o_0	o_1
0	0	0
1	1	1

Universal gates

A set of gates is **universal** if for every boolean function f, there is a reversible circuit r built from those such that f is obtained by discarding some outputs from r.

For instance,

- NOT + CNOT is not universal,
- CCNOT is universal,
- CSWAP is universal.

Reversible computing

In general, starting from a blank tape, we want our machines to give a blank tape (otherwise energy is required to reset it!) [Ben73]

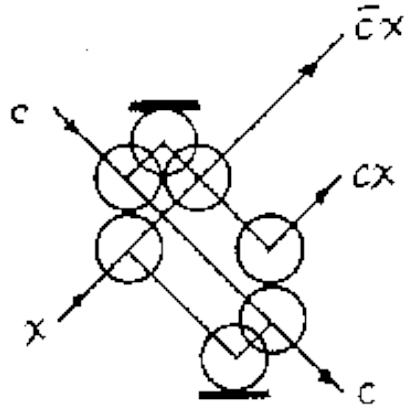
Typically, starting from a blank tap and data, we

1. perform our computation, keeping intermediate results,
2. copy the final result to some memory,
3. reverse the computation to obtain again a blank tape.

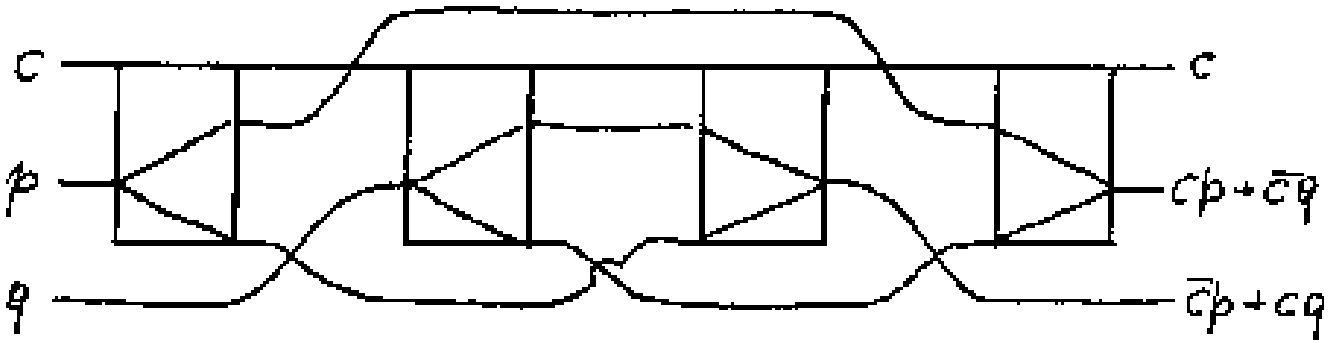
We can implement reversible computations
on physical devices!
[Ben82]

The billiard-ball model

In the billiard-ball model [FT82], the switch:



and CSWAP:



In this model, only bijections which are conservative (preserve the number of 1) can be implemented: we code a bit as a pair 01 / 10.

A chemical machine

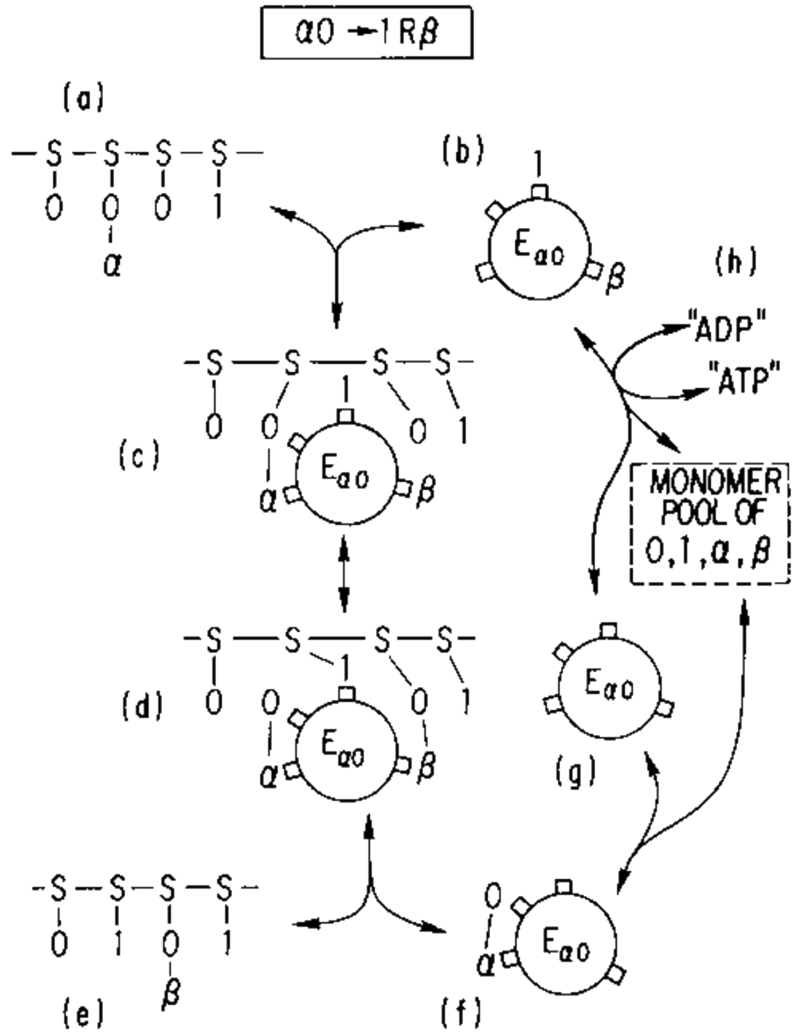


Fig. 6. Hypothetical enzymatic Turing machine. Macromolecular tape (a) consists of a structural backbone S–S–S bearing tape symbols 1,0 and head marker α. Macromolecule reacts (c,d) with enzyme (b) that catalyzes the transition $\alpha 0 \rightarrow 1R\beta$, via specific binding sites (tabs), thereby resulting in logical successor configuration (e). Enzyme is then prepared for reuse

A mechanical machine

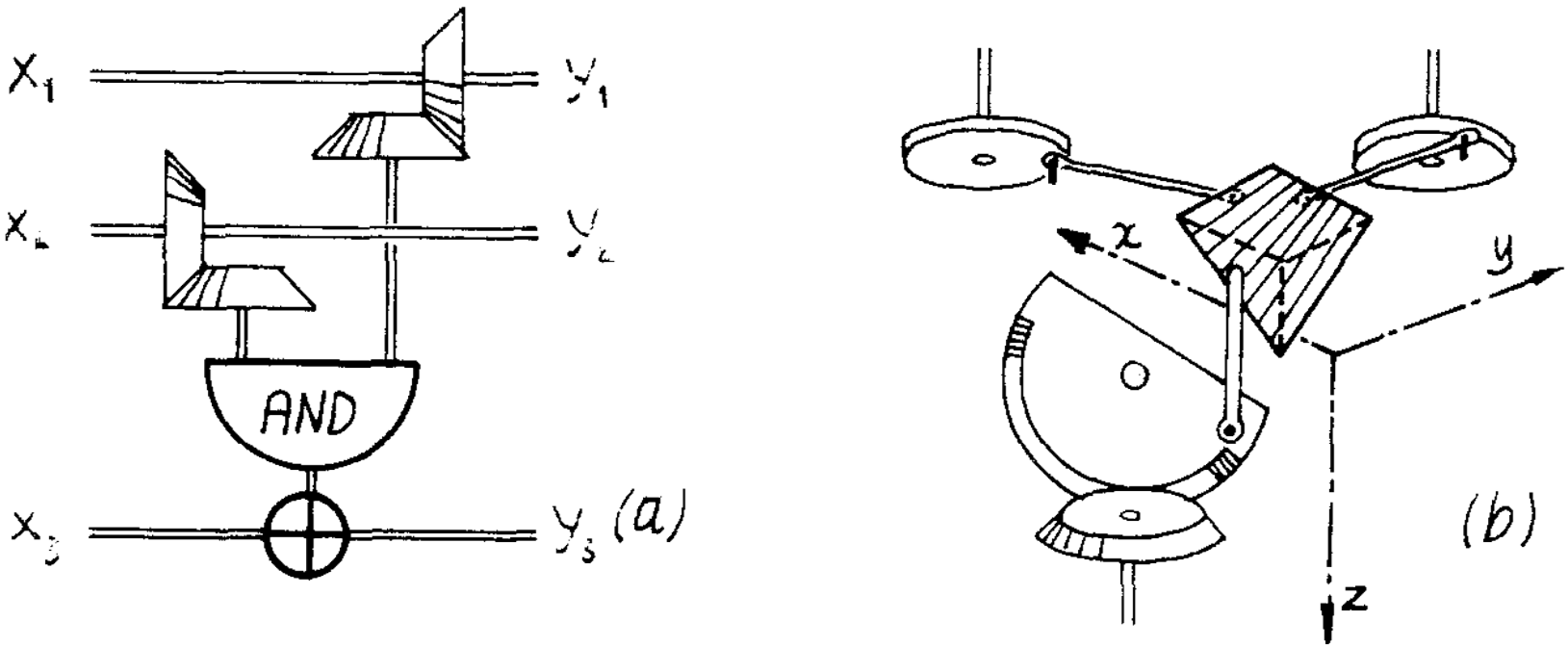


Fig. 5. (a) Realization of $\Theta^{(3)}$, (b) Details of the AND mechanism.

A mechanical machine

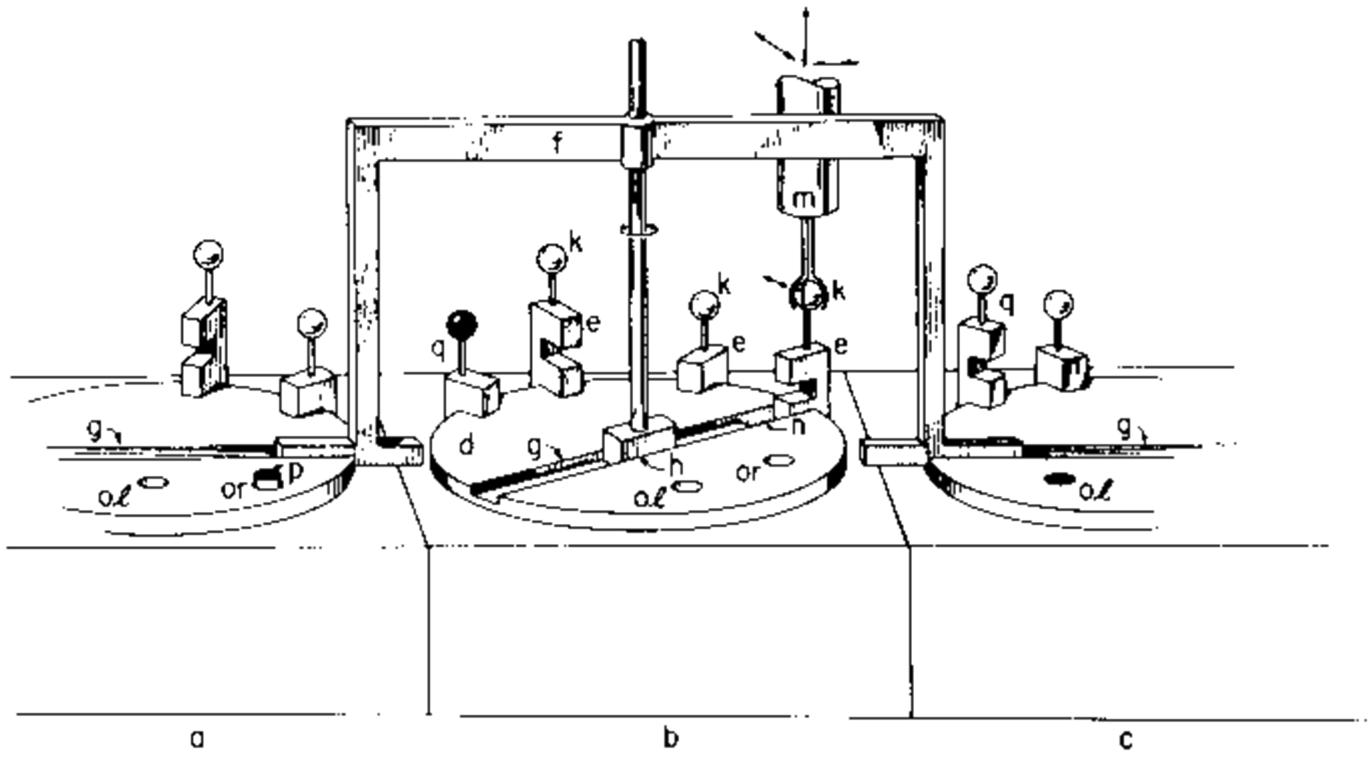


Fig. 7. Brownian Turing machine made of rigid, frictionless, loosely fitting clockwork. This figure shows the Turing machine tape (a,b,c) and the read–write–shift equipment. The machine is scanning square b. Each tape square has a disk (d) which interlocks with several E-shaped bit-storage blocks (e), holding them in the up (1) or down (0) position. A framework (f) fits over the scanned tape square, engaging the disks of the two adjacent squares (via their grooves g), to keep them from rotating when they are not supposed to. After the bits are read (cf. next figure) they must in general be changed. In order to change a bit, its knob (k) is first grasped by the manipulator (m), then the notch (n) is rotated into alignment by the screwdriver-

A mechanical machine

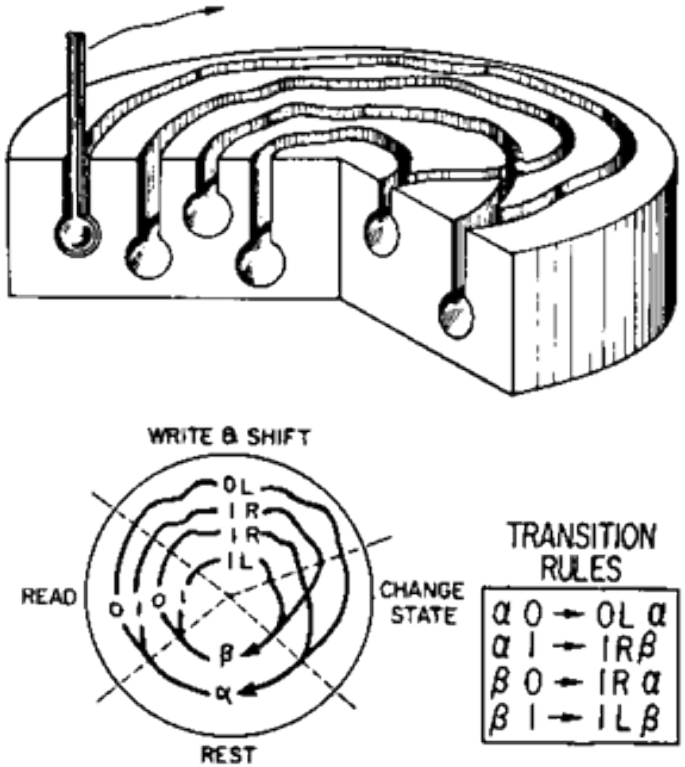


Fig. 9. Above: master camshaft of the clockwork Turing machine's control unit. Below: top view of camshaft, and the transition rules to which its tunnels are isomorphic.

Note that the brownian movement will make it move randomly, so we only need a bit of energy to push it forward. If the function was not reversible, we would get lost in possible backward paths.

Relations

We know the gates to generate boolean circuits (do we?).

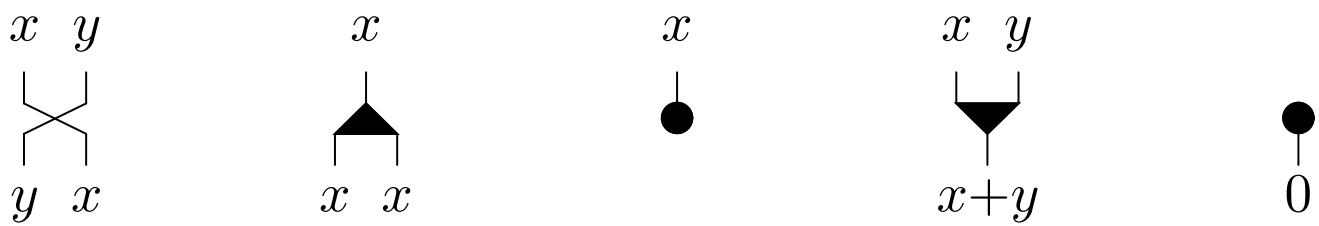
But what are the relations?

Lafont [Laf03] has investigated presentation for the corresponding PROP.

PROP = symmetric monoidal category with $\mathbb{N}$ as objects

The PROP of functions

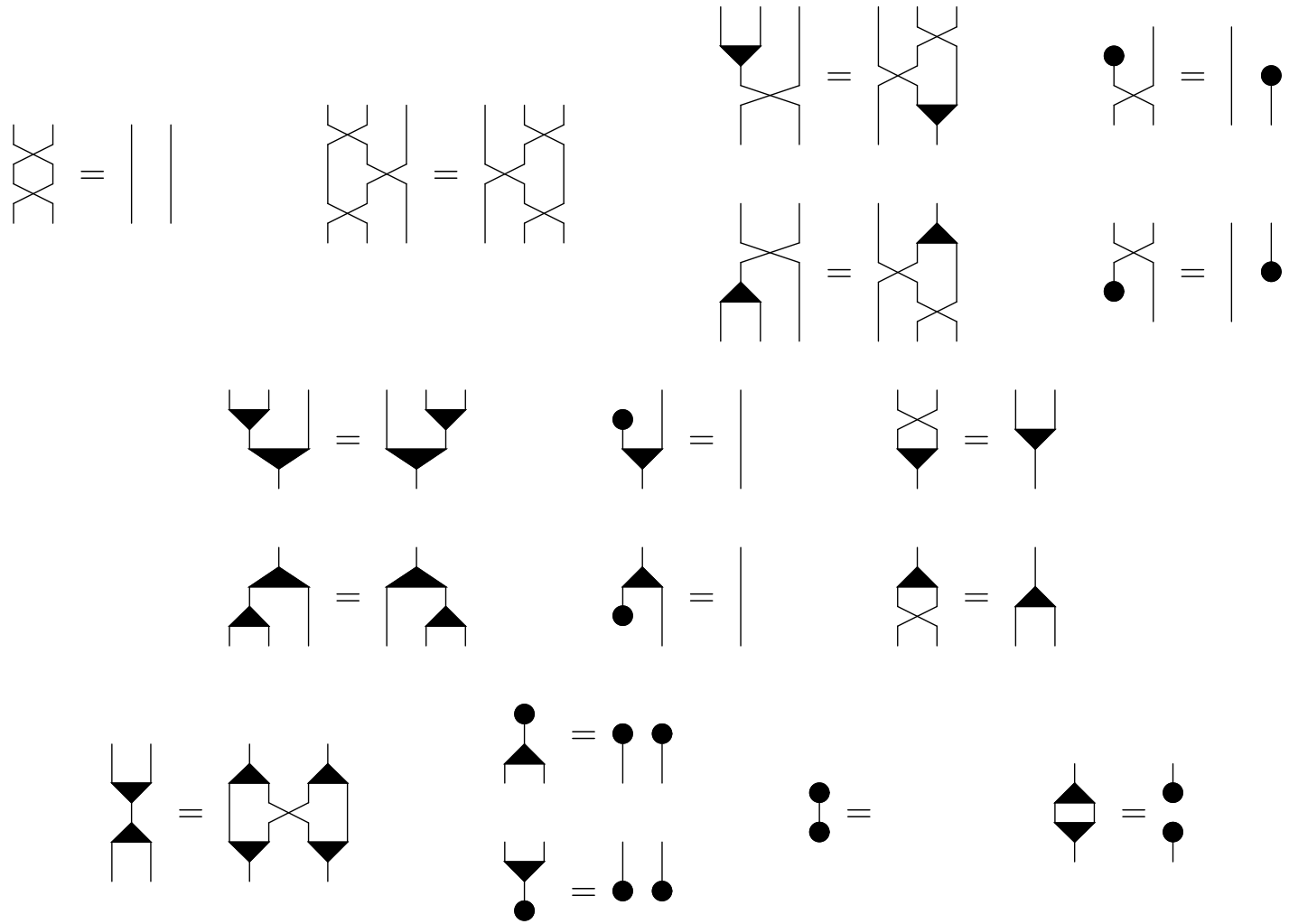
The PROP with morphisms functions $\mathbb{B}^m \to \mathbb{B}^n$ is generated by



and

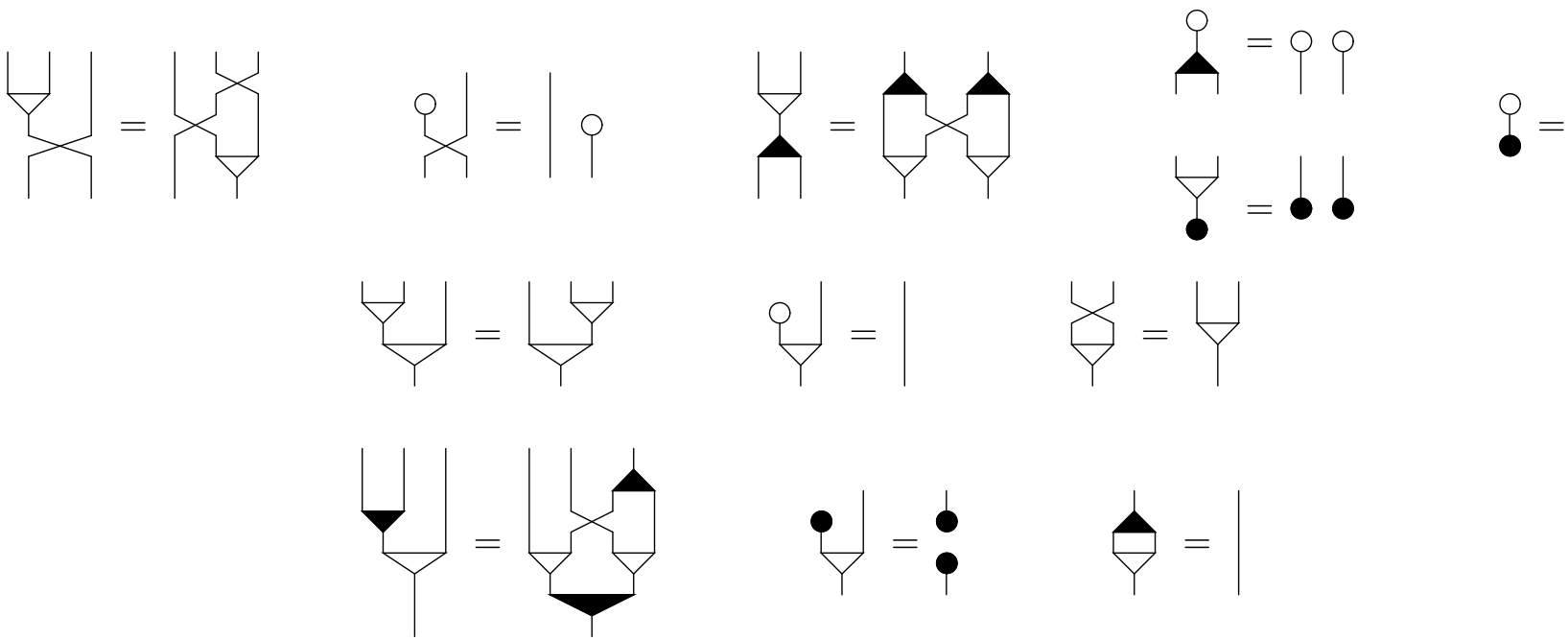
The PROP of functions

Subject to relations:



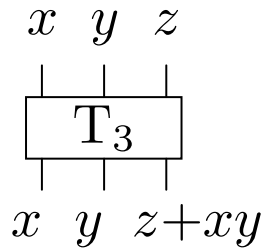
The PROP of functions

and



The PROP of boolean bijections

For the PROP **B** of boolean bijections, we could hope that it is generated by the CCNOT gate:



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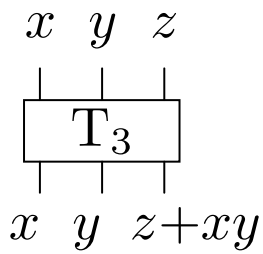

Theorem

The PROP **B** *is not finitely generated.*

Proof.

This follows from the remark that if

$$f \quad : \quad \mathbb{B}^n \quad \to \quad \mathbb{B}^n$$

is a bijection, then

$$f \times \mathrm{id}_{\mathbb{B}} \quad : \quad \mathbb{B}^{n+1} \quad \to \quad \mathbb{B}^{n+1}$$

is an even permutation. □

The PROP of boolean bijections

However,

Theorem

The PROP **A** *of even permutations is contained in the sub-PROP of* **B** *generated by* τ*,* T_1*,* T_2 *and* T_3*. It is thus finitely generated.*

The relations are not known though.

The PROP of boolean bijections

However,

Theorem

The PROP **A** *of even permutations is contained in the sub-PROP of* **B** *generated by* τ, T_1, T_2 *and* T_3. *It is thus finitely generated.*

The relations are not known though.

As a corollary, we have

Theorem

The PROP **B** *is generated by* τ *and the* T_n *for* $n \geq 1$.

The relations are not known though.

Question

Since we have duplication, we are more interested in the PROP for boolean injections.

It could also be interesting to consider conservative bijections.

I don’t know of any presentation.

Unfoldings

- RCCS
- reversing = universal cover (we take a cofibrant replacement)

There is another fundamental physical computer based on quantum mechanics.

We need some more material to appreciate it.

CLASSICAL MECHANICS

Newton's law

Recall **Newton's law** of motion

$$m\ddot{q} \quad = \quad F$$

(we write q for the position of the particle).

It can be derived from first principles!

Newton's law

Recall **Newton's law** of motion

$$\dot{p} \quad = \quad F$$

(we write $p = m\dot{q}$ for the **momentum** of the particle).

It can be derived from first principles!

Lagrangian mechanics

Axiom

Any mechanical system (e.g. a particle) is characterized by a function, called **Lagrangian**

$$L(q, \dot{q})$$

depending on

- the *position* q,
- the *velocity* $\dot{q}$,
- and not anything else (not $\ddot{q}$, a hidden variable, etc.)!

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Remark

Here $\dot{q}$ is a formal parameter (not a derivative), i.e.,

$$L \quad : \quad TQ \quad \to \quad \mathbb{R}$$

for some manifold Q.

Action

The **action** is

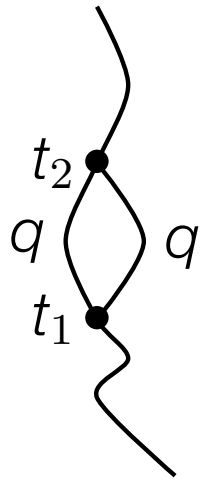
$$S = \int_{t_1}^{t_2} L(q, \dot{q})\, \mathrm{d}t$$

Axiom

The **principle of least action**: a mechanical system has minimal (or, more precisely, stationary) action.

The principle of least action

If we change q to $q + s\,\delta q$, the first-order variation of the action should be zero:



$q + s\,\delta q \qquad \rightsquigarrow \qquad \delta S = 0$

The principle of least action

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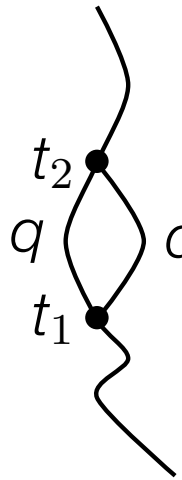


$$q + s\,\delta q \qquad \rightsquigarrow \qquad \delta S = 0$$

A **variation** of q is a function δq such that

$$\delta q(t_1) = \delta q(t_2) = 0$$

and we formally consider

$$\delta S \quad = \quad \frac{\mathrm{d}}{\mathrm{d}s} S(q_s)\Big|_{s=0}$$

with

$$q_s \quad = \quad q + s\,\delta q$$

Euler-Lagrange equation

We have

$$\begin{aligned}
\delta S &= \delta \int_{t_1}^{t_2} L \, \mathrm{d}t \\
&= \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right) \mathrm{d}t \\
&= \left[\frac{\partial L}{\partial \dot{q}} \delta q \right]_{t_1}^{t_2} + \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{q}} \right) \delta q \, \mathrm{d}t
\end{aligned}$$

(by an i.p.p. since $\delta \dot{q} = \mathrm{d}\delta q \,/\, \mathrm{d}t$).

Euler-Lagrange equation

We have

$$\begin{aligned}
\delta S &= \delta \int_{t_1}^{t_2} L \,\mathrm{d}t \\
&= \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right) \mathrm{d}t \\
&= \left[\frac{\partial L}{\partial \dot{q}} \delta q \right]_{t_1}^{t_2} + \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{q}} \right) \delta q \,\mathrm{d}t
\end{aligned}$$

(by an i.p.p. since $\delta \dot{q} = \mathrm{d}\delta q \,/\, \mathrm{d}t$).

Therefore $\delta S = 0$ for every δq if and only if

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q}$$

called the **Euler-Lagrange equation**.

The Euler-Lagrange equation

We have:

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q}$$

We define

- the **momentum**:

$$p = \frac{\partial L}{\partial \dot{q}}$$

- the **force**:

$$F = \frac{\partial L}{\partial q}$$

The equation becomes

$$\frac{\mathrm{d}p}{\mathrm{d}t} = F$$

Conservative forces

A force F is **conservative** if there is a potential $V : Q \to \mathbb{R}$ such that

$$F \quad = \quad -\frac{\partial V}{\partial q}$$

(or $F = -\nabla V$ in general).

This is equivalent to the **work**

$$V(q) \quad = \quad -\int_{q_0}^{q} F \cdot \mathrm{d}q \quad = \quad -\int_{\substack{t_1 \\ q(t_1)=q_0 \\ q(t_2)=q}}^{t_2} F(q) \cdot \dot{q}\, \mathrm{d}t$$

being well-defined, i.e., not depending on the chosen path.

We will see that energy is conserved for those.

Conservative forces

Axiom

All forces are conservative.

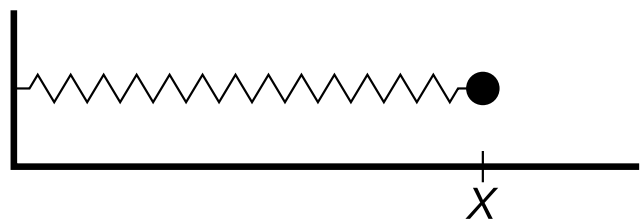
Conservative forces

Axiom

All forces are conservative.

Example

For the harmonic oscillator,



we have

$$F = -kx \qquad V = \frac{1}{2}kx^2$$

Conservative forces

Axiom

All forces are conservative.

Example

A friction force

$$F = -\alpha \dot{x}$$

is not conservative, but there are missing parts in our system!

The Lagrangian

In general, the Lagrangian looks like

$$L \quad = \quad E - V \quad = \quad \frac{1}{2} m \dot{q}^2 - V$$

so that

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{q}} \quad = \quad m\ddot{q} \quad = \quad F \quad = \quad \frac{\partial L}{\partial q}$$

We recover Newton's equation!

Conservation of energy

The laws of physics are invariant by translation in time:

$$\frac{\partial L}{\partial t} = 0$$

Therefore,

$$\begin{aligned}
\frac{\mathrm{d}L}{\mathrm{d}t} &= \frac{\partial L}{\partial q}\dot{q} + \frac{\partial L}{\partial \dot{q}}\ddot{q} + \frac{\partial L}{\partial t} \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}}\dot{q} + \frac{\partial L}{\partial \dot{q}}\ddot{q} \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}}\dot{q}\right)
\end{aligned}$$

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We define the **energy** (or **hamiltonian**) as

$$H = \frac{\partial L}{\partial \dot{q}}\dot{q} - L$$

and have

$$\frac{\mathrm{d}H}{\mathrm{d}t} = 0$$

Noether's theorem

Theorem

If there is a continuous symmetry of the system then there is a conserved quantity.

Noether's theorem

Theorem

If there is a continuous symmetry of the system then there is a conserved quantity.

We suppose given a map

$$\begin{array}{rcl} Q^{\mathbb{R}} \times \mathbb{R} & \to & Q^{\mathbb{R}} \\ (q, s) & \mapsto & q_s \end{array}$$

Typically,

$$q_s(t) = q(t+s) \qquad q_s(t) = q(t) + sv \qquad \text{etc.}$$

Consider and infinitesimal transformation and its effect on S:

$$\delta q = \frac{\mathrm{d}}{\mathrm{d}s} q_s \Big|_{s=0} \qquad \delta L = \frac{\mathrm{d}}{\mathrm{d}s} S(q_s, \dot{q}_s) \Big|_{s=0}$$

Noether's theorem

We have (we already went through this)

$$\begin{aligned} \delta S &= \dots \\ &= \left[\frac{\partial L}{\partial \dot{q}}\delta q\right]_{t_1}^{t_2} + \int_{t_1}^{t_2} \underbrace{\left(\frac{\partial L}{\partial q} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}}\right)}_{=0} \delta q \, \mathrm{d}t \end{aligned}$$

Therefore $\delta S = 0$ implies that the quantity

$$\frac{\partial L}{\partial \dot{q}}\delta q = p\delta q$$

is invariant with respect to t.

Noether's theorem

More generally, if

$$\delta L = \frac{\mathrm{d}\ell}{\mathrm{d}t}$$

then the quantity

$$p\,\delta q - \ell$$

is conserved over time.

Noether's theorem

A general galilean transformation is given by

$$\begin{aligned} \mathbf{x} &\rightsquigarrow \mathbf{x}' = R\mathbf{x} + \mathbf{a} + \mathbf{v}t \\ t &\rightsquigarrow t' = t + s \end{aligned}$$

symmetry	invariant
translation in time (s)	energy (hamiltonian)
translation in space ($\mathbf{a}$)	momentum
uniform move ($\mathbf{v}$)	center of mass
rotation (R)	angular momentum
gauge invariance of the e.m. field	conservation of charge
⋮	⋮

Reversibility

There is another kind of symmetry which is not covered:

$$\begin{aligned} q &\mapsto q \\ \dot{q} &\mapsto -\dot{q} \\ t &\mapsto -t \end{aligned}$$

Time is reversible!

In fact, since the evolution is described by a differential equation it is **reversible**: two states cannot lead to the same state.

Parity inversion

If we negate all the coordinates, i.e.,

$$q \quad \rightsquigarrow \quad -q$$

This generally gives rise to a discrete symmetry, but is violated in weak interactions (Wu experiment)!

Hamiltonian mechanics

In Lagrangian mechanics, everything is indexed in $(q, \dot{q}) \in TQ$.

We can also use the **phase space** $(q, p) \in T^*Q$.

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which is valid if

$$\det\left(\frac{\partial p_i}{\partial \dot{q}_j}\right) = \det\left(\frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j}\right) \quad \neq \quad 0$$

Hamiltonian mechanics

Hamilton's equations are satisfied:

$$\frac{\mathrm{d}q}{\mathrm{d}t} = \frac{\partial H}{\partial p} \qquad \frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H}{\partial q}$$

(the second by Euler-Lagrange)

The Poisson bracket

Given $A, B : T^*Q \to \mathbb{R}$, their **Poisson bracket** is

$$\{A, B\} \quad = \quad \sum_i \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i}$$

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This is a Lie bracket:

- linear
- antisymmetric: $\{B, A\} = -\{A, B\}$
- satifying Jacobi: $\{\{A, B\}, C\} + \{\{B, C\}, A\} + \{\{C, A\}, B\} = 0$

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In particular

$$\{q_i, q_j\} = \{p_i, p_j\} = 0 \qquad\qquad \{q_i, p_j\} = \delta_{ij}$$

hamiltonian = evolution

The hamiltonian encodes the evolution of a physical quantity $A : T^*Q \to \mathbb{R}$:

$$\begin{aligned} \frac{\mathrm{d}A}{\mathrm{d}t} &= \frac{\mathrm{d}A}{\mathrm{d}q}\frac{\mathrm{d}q}{\mathrm{d}t} + \frac{\mathrm{d}A}{\mathrm{d}p}\frac{\mathrm{d}p}{\mathrm{d}t} \\ &= \frac{\mathrm{d}A}{\mathrm{d}q}\frac{\partial H}{\partial p} - \frac{\mathrm{d}A}{\mathrm{d}p}\frac{\partial H}{\partial q} \\ &= \{A, H\} \end{aligned}$$

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In particular, Hamilton equations are

$$\frac{\mathrm{d}q}{\mathrm{d}t} = \{q, H\} \qquad \frac{\mathrm{d}p}{\mathrm{d}t} = \{p, H\}$$

TODO: Noether's theorem.....

QUANTUM MECHANICS

Hilbert spaces

A Hilbert space $\mathcal{H}$ is a $\mathbb{C}$-vector space equipped with an *inner product* such that

- $\langle \phi | - \rangle$ is linear
- $\langle - | \psi \rangle$ is antilinear
- $\langle \phi | \psi \rangle = \langle \psi | \phi \rangle^*$
- $\langle \psi | \psi \rangle \geq 0$

We write

- $\|\psi\| = \sqrt{\langle \psi | \psi \rangle}$ for the norm
- $|\psi\rangle \in \mathcal{H}$ for a vector
- $\langle \psi | = \langle \psi | - \rangle \in \mathcal{H}^*$

Hilbert spaces

The bra-ket notation is nice:

$$\langle\phi|\ |\psi\rangle \quad = \quad \langle\phi|\psi\rangle$$

and more generally, for $A : \mathcal{H} \to \mathcal{H}$

$$\langle A^*\phi|\psi\rangle \quad = \quad \langle\phi|\,A\,|\psi\rangle \quad = \quad \langle\phi|A\psi\rangle$$

where A^* is the conjugate transpose of A:

$$\langle\phi|\,A\,|\psi\rangle \quad = \quad \langle\psi|\,A^*\,|\phi\rangle$$

Hilbert spaces

An Hilbert space $\mathcal{H}$ admits an orthonormal basis (e_i):

$$\langle e_i | e_j \rangle \quad = \quad \delta_{ij}$$

- a vector:

$$|\psi\rangle \quad = \quad \sum_i \psi_i \, |e_i\rangle$$

- an operator $A : \mathcal{H} \to \mathcal{H}$

$$A_{ij} \quad = \quad \langle e_j | \, A \, | e_i \rangle$$

and

$$A \quad = \quad \sum_{i,j} |e_j\rangle \, A_{ij} \, \langle e_i|$$

Hilbert spaces

We do as if we were in finite-dimensional spaces (and trust smart people for details).

This is not a good idea since a basis for our space typically consists in all possible states $q \in Q$, or all possible values for momentum.

Self-adjoint operators

An operator A is self-adjoint when

$$A \quad = \quad A^*$$

This implies that

- its eigenvalues are real
- eigenvectors with distinct eigenvalues are orthogonal
- we can find an orthonormal basis of eigenvectors[2]

[2] in good cases (e.g. finite dimension)

Quantum mechanics

In quantum mechanics, the state of a system is given by a vector

$$|\psi\rangle$$

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$$A$$

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$$\langle A \rangle \quad = \quad \mathrm{tr}(|\psi\rangle \langle\psi| A) \quad = \quad \langle\psi| A |\psi\rangle$$

(supposing $\langle\psi|\psi\rangle = 1$, otherwise divide by it)

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(supposing $\langle\psi|\psi\rangle = 1$, otherwise divide by it) where

$$|\psi\rangle\langle\psi|$$

is the **density operator** associated to $|\psi\rangle$.

Density operators

Note that we only care about the density operator

$$\rho \quad = \quad |\psi\rangle \langle\psi|$$

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$$\rho \quad = \quad |\psi\rangle \langle\psi|$$

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More generally, we can consider as a **density operators** any ρ which is self-adjoint, nonnegative ($\langle\psi| \rho |\psi\rangle \geq 0$) and of unit trace, those as above are *pure states*.

Expectation generalizes as expected

$$\langle A \rangle \quad = \quad \frac{\mathrm{tr}(\rho A)}{\mathrm{tr}\, \rho}$$

Symmetries

A *symmetry* for a system has to preserve inner product and thus be of the form

$$\begin{aligned} |\psi\rangle &\mapsto U|\psi\rangle \\ A &\mapsto UAU^* \end{aligned}$$

for some **unitary** transformation U

$$UU^* = U^*U = I$$

Remark

Most operations are (sub)unitary because we want to preserve normalization of states: $\langle\psi|\psi\rangle = 1$.

Symmetries

Consider a continuous family of transformations $U(s)$ such that

$$U(0) = I \qquad\qquad U(s_1 + s_2) = U(s_1)U(s_2)$$

The associated *infinitesimal transformation* is

$$\delta U \quad = \quad \left.\frac{\mathrm{d}U}{\mathrm{d}s}\right|_{s=0}$$

i.e.,

$$U \quad = \quad I + s\,\delta U + O(s^2)$$

By unitarity, we have

$$I \quad = \quad UU^* \quad = \quad I + s(\delta U + \delta U^*) + O(s^2)$$

thus

$$\delta U + \delta U^* \quad = \quad 0$$

and therefore

$$\delta U \quad = \quad iK$$

for some self-adjoint (real) K.

It determines U since

$$\left.\frac{\mathrm{d}U(s_0+s)}{\mathrm{d}s}\right|_{s=0} = \delta(U(s_0+s)) = \delta(U(s_0)U(s)) = U(s_0)\,\delta U$$

thus

$$\left.\frac{\mathrm{d}U(s)}{\mathrm{d}s}\right|_{s=s_0} = U(s_0)\,\mathrm{i}K$$

i.e.,

$$\frac{\mathrm{d}U}{\mathrm{d}s} = U\,\mathrm{i}K$$

thus

$$U = \mathrm{e}^{\mathrm{i}Ks}$$

Operators from symmetries

A general galilean transformation is

$$\begin{aligned} \mathbf{x} &\rightsquigarrow \mathbf{x}' = R\mathbf{x} + \mathbf{a} + \mathbf{v}t \\ t &\rightsquigarrow t' = t + s \end{aligned}$$

symmetry	operator
rotation	$e^{-i\theta_k J_k}$
translation	$e^{-ia_k P_k}$
velocity	$e^{iv_k G_k}$
time	e^{isH}

Note: we should divide all operators by $\hbar$ but nevermind.

Evolution in time

A translation in time

$$t \quad \rightsquigarrow \quad t' = t + s$$

induces a transformation of a vector

$$|\psi(t)\rangle \quad \rightsquigarrow \quad |\psi'(t)\rangle = |\psi(t-s)\rangle = \mathrm{e}^{\mathrm{i}sH} |\psi(t)\rangle$$

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which is solution of **Schrödinger's equation**

$$\frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle \quad = \quad -\mathrm{i}H |\psi(t)\rangle$$

or even

$$H \quad = \quad \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}$$

Evolution in time

The **position operator** Q is

$$Q\,|x\rangle = x\,|x\rangle$$

Evolution in time

The **position operator** Q is

$$Q\,|x\rangle = x\,|x\rangle$$

The **velocity operator** V has to satisfy

$$\langle V\rangle \quad = \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle Q\rangle$$

and thus

$$\begin{aligned}\langle\psi|\,V\,|\psi\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\left(\langle\psi|\,Q\,|\psi\rangle\right) &= \left(\frac{\mathrm{d}}{\mathrm{d}t}\,\langle\psi|\right)Q\,|\psi\rangle + \langle\psi|\,Q\left(\frac{\mathrm{d}}{\mathrm{d}t}\,|\psi\rangle\right)\\ &= \mathrm{i}\,\langle\psi|\,HQ\,|\psi\rangle - \mathrm{i}\,\langle\psi|\,QH\,|\psi\rangle\end{aligned}$$

i.e.,

$$V \quad = \quad \mathrm{i}(HQ - QH) \quad = \quad \mathrm{i}[H, Q]$$

Pictures of motion

The Heisenberg equation of motion is

$$\mathrm{i}\frac{\mathrm{d}A}{\mathrm{d}t} = [A, H]$$

whose solution is

$$A(t) \quad = \quad U^{-1}(t)A(0)U(t)$$

with $U(t) = \mathrm{e}^{-\mathrm{i}Ht}$.

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In the **Heisenberg picture**

$$\langle A \rangle \quad = \quad \langle \psi | \left(U^{-1} A_0 U \right) | \psi \rangle$$

In the **Schrödinger picture**

$$\langle A \rangle \quad = \quad \left(\langle \psi | U^{-1} \right) A_0 \left(U | \psi \rangle \right)$$

Noether's theorem

Given a bounded self-adjoint operator O,

$$[O, H] \quad = \quad 0$$

if and only if for every state $|\psi\rangle$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle \quad = \quad -\mathrm{i}H |\psi(t)\rangle$$

the expected value

$$\langle \psi(t) | O | \psi(t) \rangle$$

is constant.

Propagators

The evolution of the state is given by

$$|\psi(t)\rangle \quad = \quad U(t, t_0)\,|\psi(t_0)\rangle$$

and we have

$$|\psi(x, t)\rangle \quad = \quad \int \langle x|\, U(t, t_0)\,|x_0\rangle\, \psi(x_0, t_0)\, \mathrm{d}x_0$$

where the **propagator**

$$G(x, t, x_0, t_0) \quad = \quad \langle x|\, U(t, t_0)\,|x_0\rangle$$

is (proportional to) the probability of finding the particle in x at time t if it was in x_0 at t_0.

Feynman's formula

The propagator can be expressed as a *path integral*

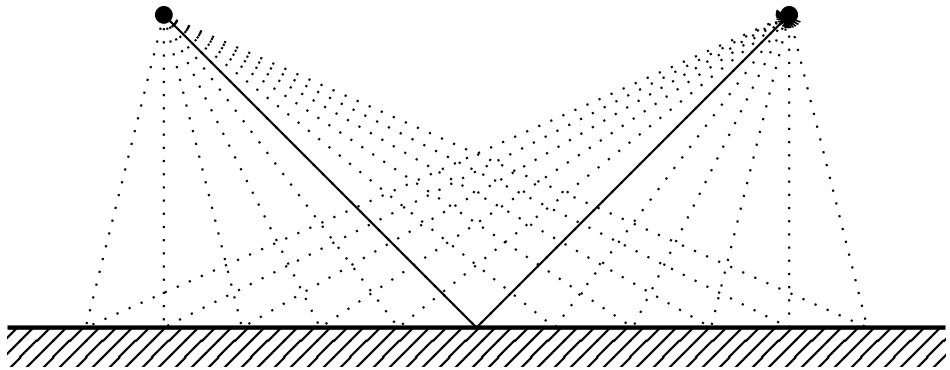
$$G(x, t, x_0, t_0) \quad = \quad \int_{\substack{q \text{ path} \\ \text{from } (x_0, t_0) \\ \text{to } (x, t)}} e^{iS(q)/\hbar}$$

where S is the **action**

$$S(q) \quad = \quad \int L(q, \dot{q})\, dt$$

The least action principle

How does light knows where the shortest path is?



(and also even more wired paths)

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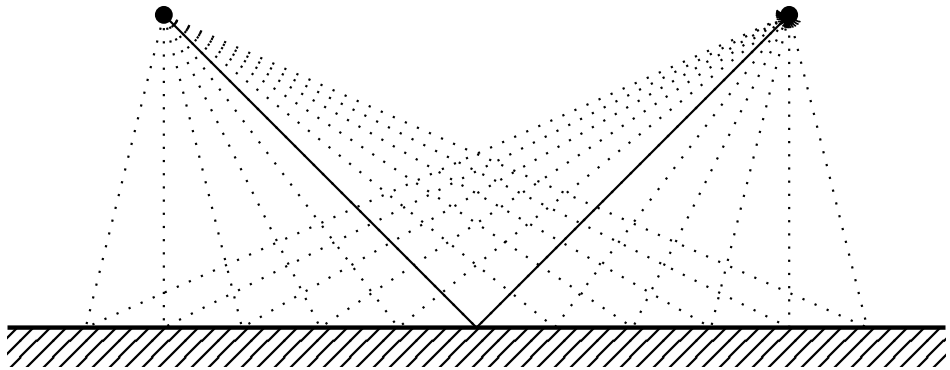

(and also even more wired paths)

It does not, it tries everything:

$$G(x,t,x_0,t_0) \quad = \quad \int \mathrm{e}^{\mathrm{i}S(q)/\hbar}\,\mathrm{D}q$$

However, the phases are pretty much random, excepting when S is stable: we have recovered the least action principle!

Quantizing physics

When quantizing the laws of physics

- we replace functions by operators
- the Poisson brackets become commutators

$$[Q_i, Q_j] = [P_i, P_j] = 0 \qquad [Q_i, P_j] = \mathrm{i}\hbar\delta_{ij}$$

- etc.

The momentum coordinates

.....

The harmonic oscillator

Let's work out a bit the classical harmonic oscillator where

$$H = \frac{P^2}{2m} + \frac{1}{2} m\omega^2 Q^2$$

The harmonic oscillator

Let's work out a bit the classical harmonic oscillator where

$$H = \frac{P^2}{2m} + \frac{1}{2} m\omega^2 Q^2$$

We introduce the **creation** and **anihilation operators**

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(Q + \frac{1}{m\omega} \mathrm{i} P \right) \qquad a^* = \sqrt{\frac{m\omega}{2\hbar}} \left(Q - \frac{1}{m\omega} \mathrm{i} P \right)$$

and the **number operator**

$$N = a a^*$$

The harmonic oscillator

The Hamiltonian is

$$H = \frac{1}{2}\hbar\omega\left(aa^* + a^*a\right) = \hbar\omega\left(aa^* - \frac{1}{2}\right) = \hbar\omega\left(N - \frac{1}{2}\right)$$

The harmonic oscillator

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From $[Q, P] = \mathrm{i}$ follows

$$[a, a^*] = 1 \qquad [N, a] = -a \qquad [N, a^*] = a$$

The harmonic oscillator

Given an eigenvector $|n\rangle$ of N of eigenvalue $n \in \mathbb{R}$, i.e.,

$$N|n\rangle \quad = \quad n|n\rangle$$

we have

$$Na|n\rangle \quad = \quad a(N-I)|n\rangle \quad = \quad (n-1)a|n\rangle$$

We have constructed an eigenvector for the value $n-1$.

The harmonic oscillator

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We have constructed an eigenvector for the value $n-1$.

However,

$$n \quad = \quad \langle n|N|n\rangle \quad = \quad \langle a|a^*|n\rangle \quad \geq \quad 0$$

Therefore the smallest eigenvalue can only be $|0\rangle$.

The harmonic oscillator

Therefore, the eigenvectors for the hamiltonian are

$$H|n\rangle \quad = \quad E_n|n\rangle$$

with

$$E_n \quad = \quad \hbar\omega\left(n+\frac{1}{2}\right)$$

with $n \in \mathbb{N}$: energy levels are quantified.

The harmonic oscillator

Note that the relation

$$[a, a^*] \quad = \quad aa^* - a^*a \quad = \quad 1$$

means

$$\sum_n ((n+1)-1) - \sum_n ((n-1)+1) \quad = \quad 1$$

HAMILTONIAN FOR PROGRAMS

Truth values

Consider one of the following possible rings of *truth values*:

- classical: $\mathbb{B}$
- probabilistic: $[0, 1]$
- stochastic: $\mathbb{N}$
- chemical: $\mathbb{R}$
- quantum: $\mathbb{C}$

States

Consider a boolean circuit with m inputs and n outputs.

A **state** $|\psi\rangle$ is an element of $\mathbb{k}^{2^m}$:

$$\begin{aligned}
(i_0, i_1, i_2, \ldots) = (0, 0, 0, \ldots) &\quad \rightsquigarrow \quad 1 \\
(i_0, i_1, i_2, \ldots) = (1, 0, 0, \ldots) &\quad \rightsquigarrow \quad 1 \\
(i_0, i_1, i_2, \ldots) = (1, 1, 0, \ldots) &\quad \rightsquigarrow \quad 0 \\
\vdots &\quad \rightsquigarrow \quad \vdots
\end{aligned}$$

Hamiltonians

The **hamiltonian** of a boolean function

$$\mathbb{B}^m \quad \to \quad \mathbb{B}^n$$

is a linear function

$$\Bbbk^{2^m} \quad \to \quad \Bbbk^{2^n}$$

represented by a $2^m \times 2^n$-matrix.

For instance NOT:

	0	1
0	0	1
1	1	0

Operators

We define

- the **creation operator**

$$a = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad a|0\rangle = |1\rangle \quad a|1\rangle = 0$$

- the **destruction operator**

$$a^* = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad a|0\rangle = 0 \quad a|1\rangle = |0\rangle$$

- the **number operator**

$$N_a = aa^* = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \qquad N_a|0\rangle = 0|0\rangle \quad N_a|1\rangle = 1|1\rangle$$

Satisfying

$$aa^* + a^*a = 1$$

Hamiltonians

The hamiltonian associated to NOT is

$$a + a^*$$

Hamiltonians

The hamiltonian associated to NOT is

$$a + a^*$$

The hamiltonian associated to CNOT is

$$\mathrm{NOT}_b N_a + (I - N_a) \quad = \quad (b + b^*)aa^* + a^*a$$

Namely,

```
if a=1 then { b=not b }
if a=0 then {}
```

Hamiltonians

Traces (= feedback) correspond to taking exponentials.

THE GEOMETRY OF INTERACTION

Hamiltonian for programs

- Hamiltonian of a program
- GoI, execution formula (cf Abramsky, Ian Mackie)

STOCHASTIC MECHANICS

TODO: Baez stochastic

Dictionary

physics	programming
physical system	program
tangent bundle TQ	control flow graph (+ states)
speed $\dot{q}$	instruction

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