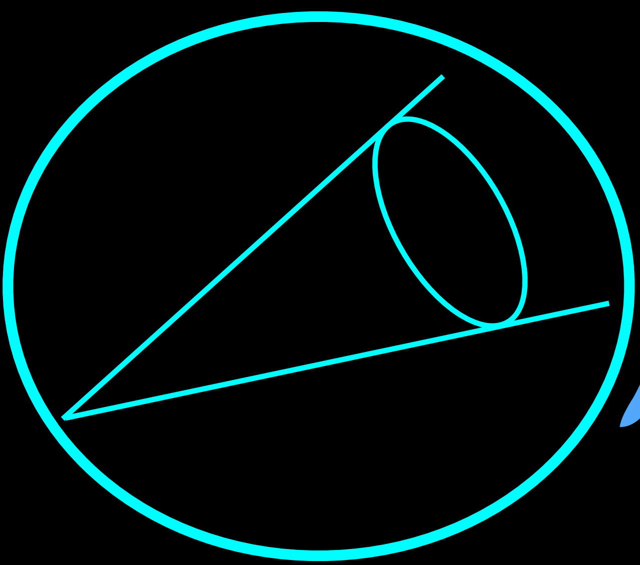
Before we start…

In memory of Chris King

† 15 March 2023



$P(uv\ldots w)$

Hidden Markov Models: Classical, Quantum, and Beyond

Andreas Winter

(with A. Monras, M. Fanizza & J. Lumbreras)

[A. Monràs/AW, JMP 57:015219 (2016), arXiv:1412.3634;
M. Fanizza/J. Lumbreras/AW, arXiv:2209.11225]

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Assume stationarity, i.e. for all t and ℓ,

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These marginals $P(\underline{u})$, for all finite words

$$\underline{u} = u_1 u_2 \ldots u_\ell \in \mathbb{M}^* = \bigcup_{k \geq 0} \mathbb{M}^k,$$

determine the probability law.

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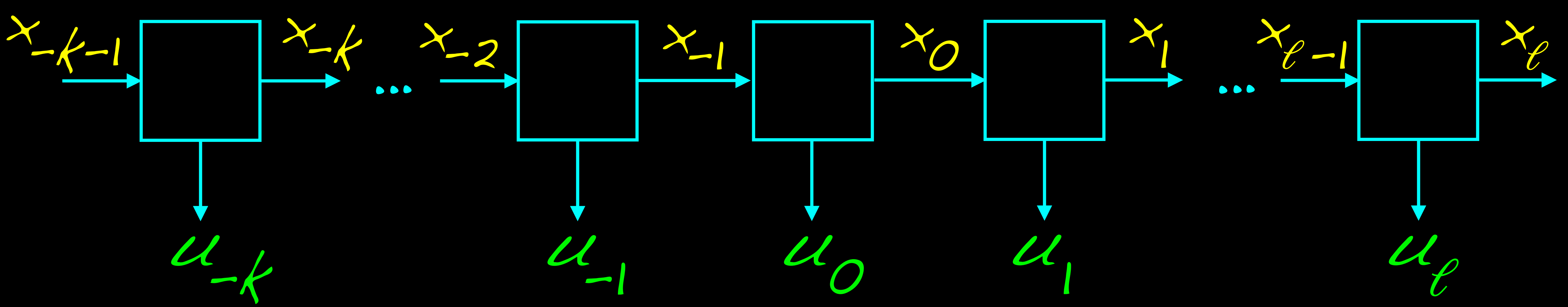
"Explanation" of $P(\underline{u})$ via a finite memory system as hidden cause:



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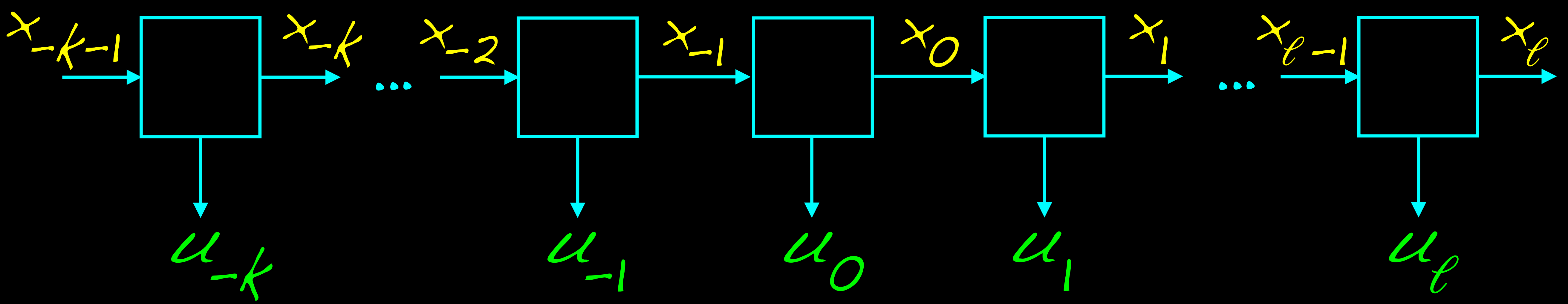
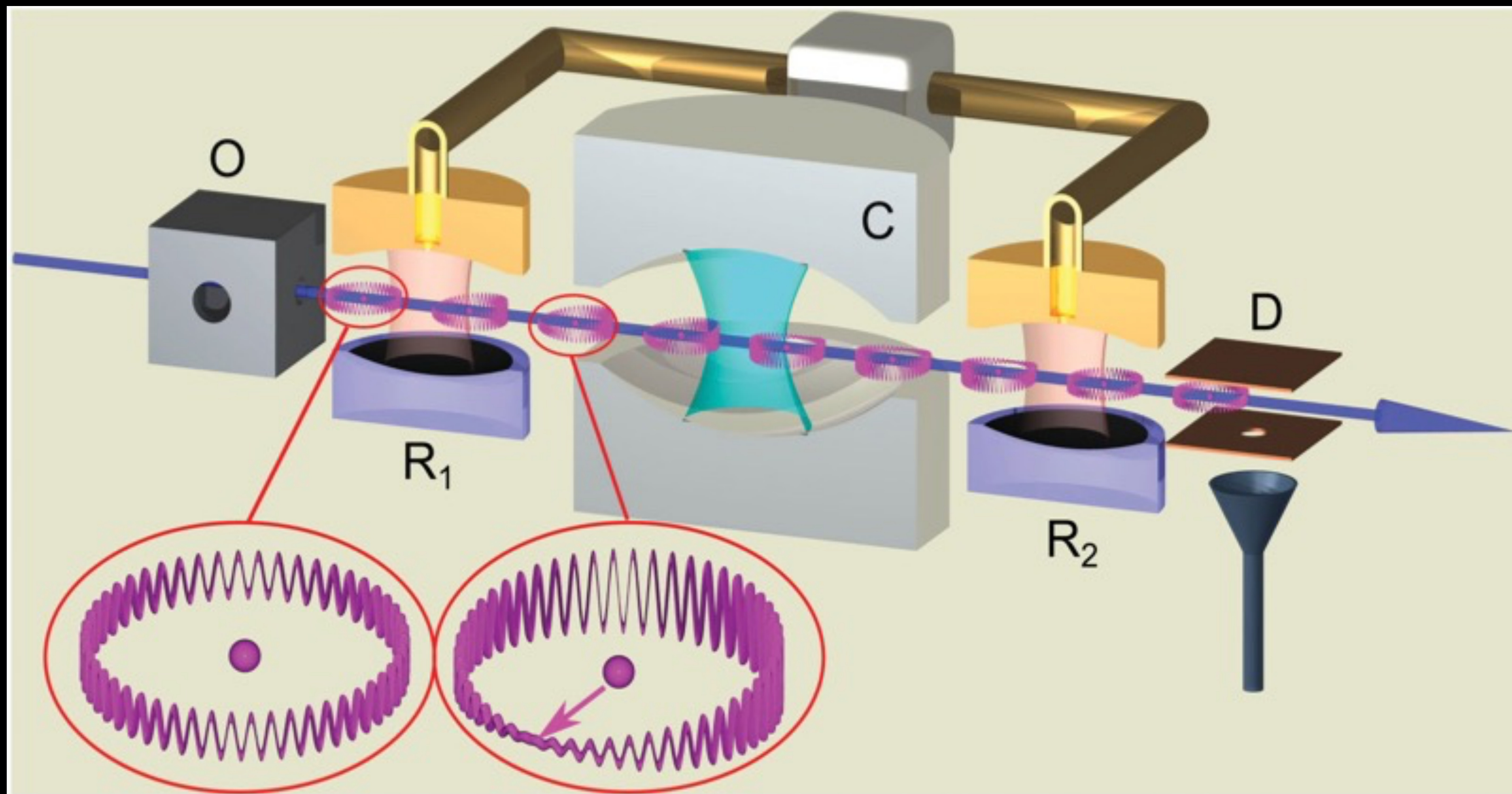


Of course, need to specify the nature of the causation, and of the memory...

Example: Cavity-atom interaction

[Courtesy of S. Haroche]:



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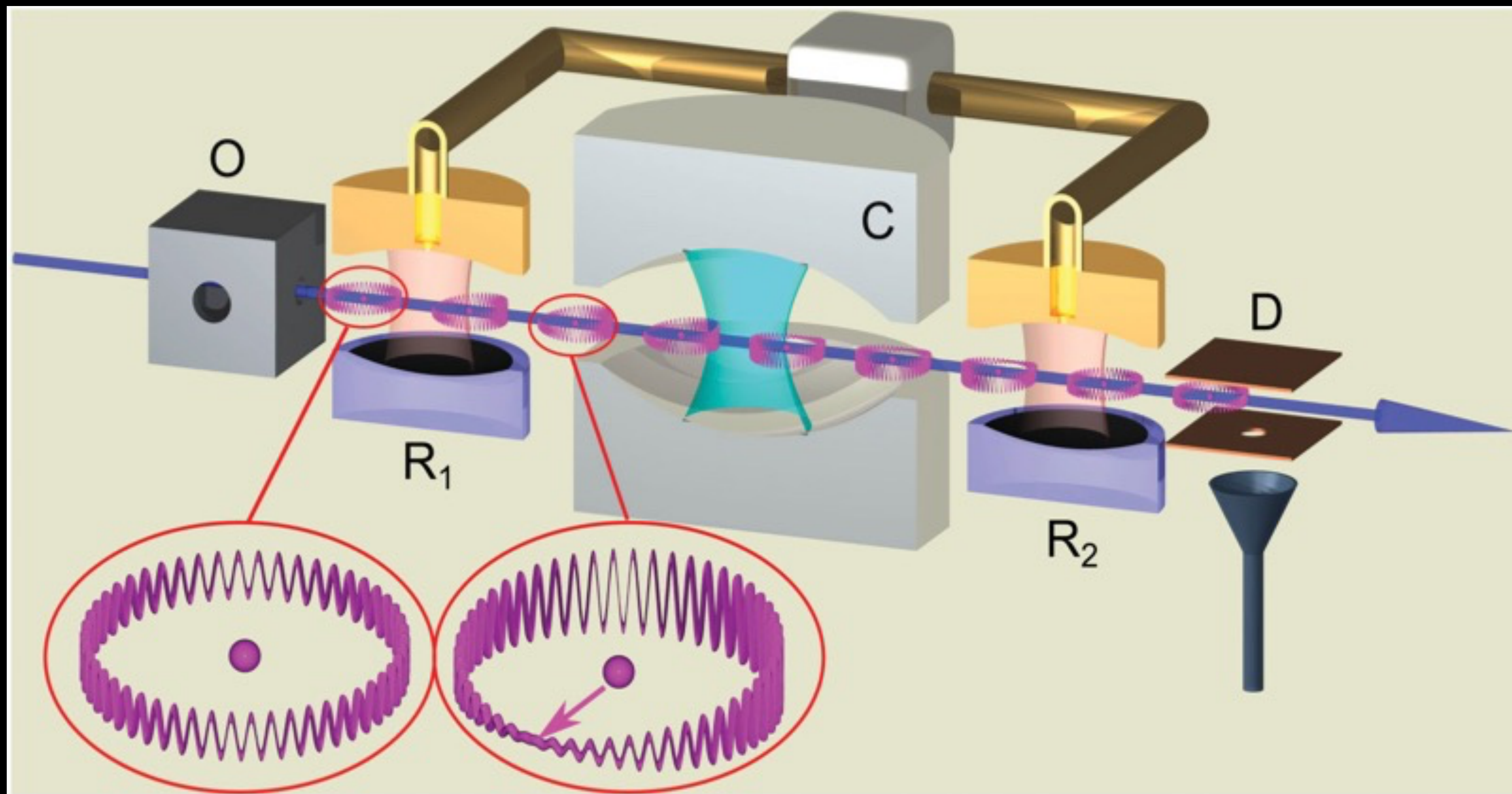


Question: can one infer the quantum nature of the internal mechanism by observing $P(\underline{u})$?

Outline

√. Observations as consequence of a finitary hidden cause (memory)

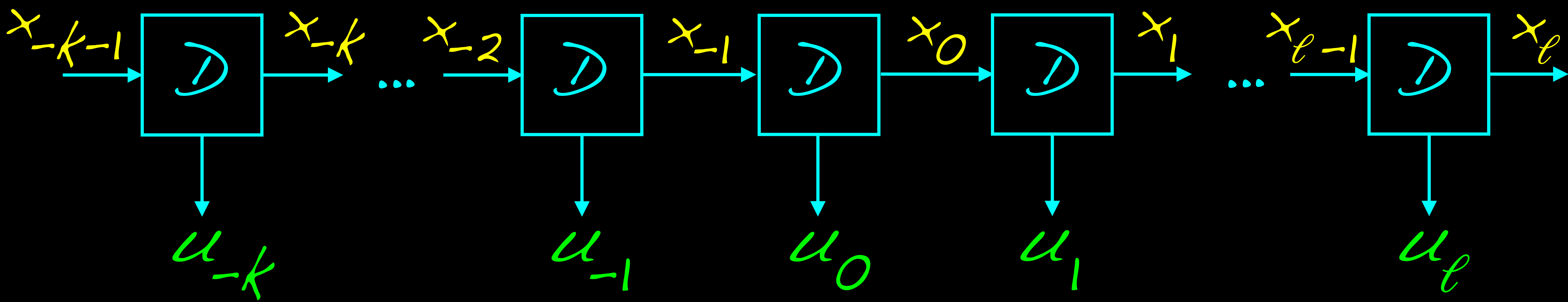
1. Classical, quantum and GPT memory

2. Reconstructing a quasi-realisation: low-rank Hankel matrix completion

3. Separations: classical $\overset{\checkmark}{\subsetneq}$ quantum $\overset{\checkmark}{\subsetneq}$ GPT

I-a. Classical memory (HMM)

The $x_t \in \mathbb{X}$ are from a finite set of internal states, $\mathcal{D}: \mathbb{X} \to \mathbb{X} \times \mathbb{M}$ are stochastic maps:

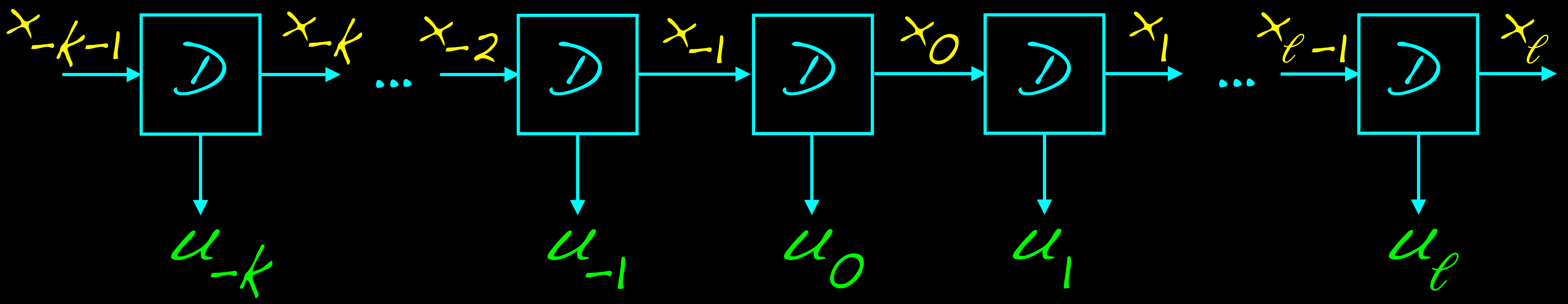


$\mathcal{D}_u : \mathbb{X} \to \mathbb{X}$ are sub-stochastic maps, s.t.
$\overline{\mathcal{D}} = \sum_u \mathcal{D}_u$ is stochastic with stationary distribution π: $\overline{\mathcal{D}}\vec{\mathbf{1}} = \vec{\mathbf{1}}$, $\pi\overline{\mathcal{D}} = \pi$.

$$P(u_1 u_2 \dots u_\ell) = \pi \mathcal{D}_{u_1} \mathcal{D}_{u_2} \cdots \mathcal{D}_{u_\ell} \vec{\mathbf{1}} \qquad \text{(p.r.)}$$

1-6. Quantum memory (HQMM)

The $x_t \in \mathbb{X} = S(\mathcal{H})$ are quantum states on $\mathcal{H}$, and $\mathcal{D}$ is a completely positive instrument:



$\mathcal{D}_u : \mathbb{X} \to \mathbb{X}$ are completely positive maps, s.t. $\bar{\mathcal{D}} = \sum_u \mathcal{D}_u$ is unital (cpup) with stationary state ω: $\bar{\mathcal{D}}\mathbb{1} = \mathbb{1}$, $\omega \circ \bar{\mathcal{D}} = \omega$.

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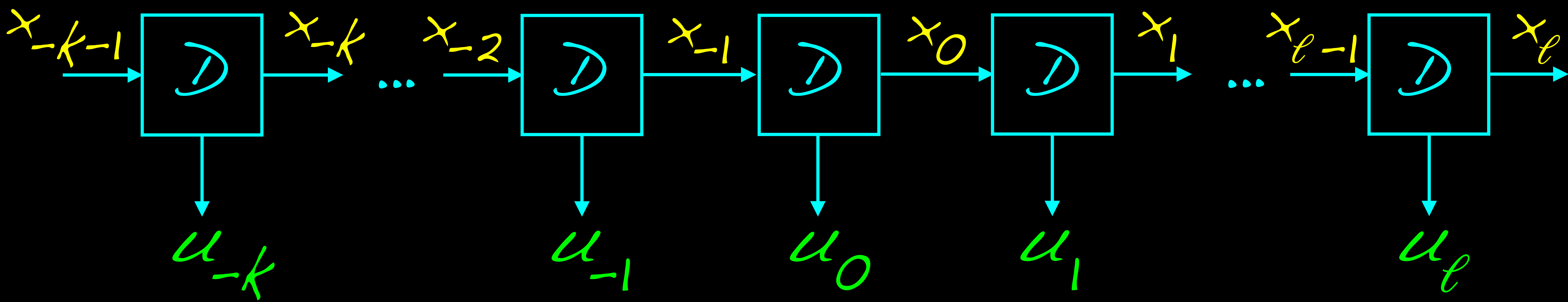

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C*-finitely correlated state

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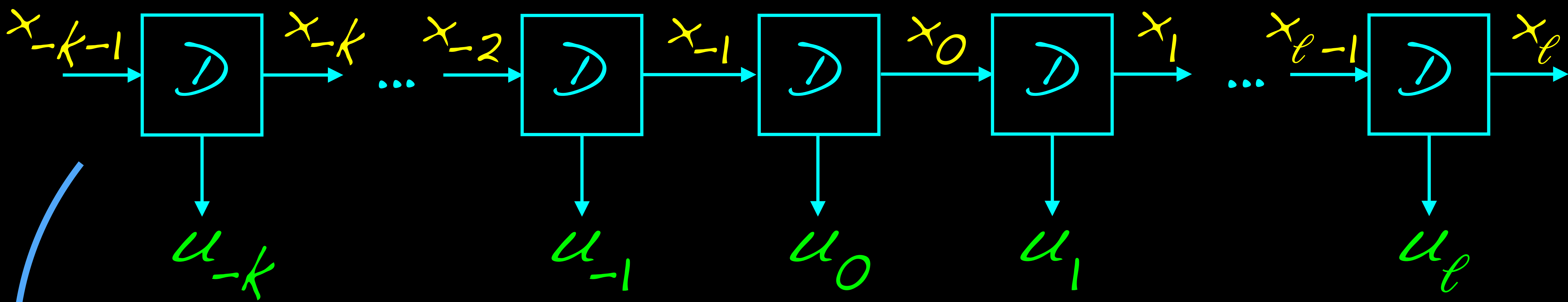
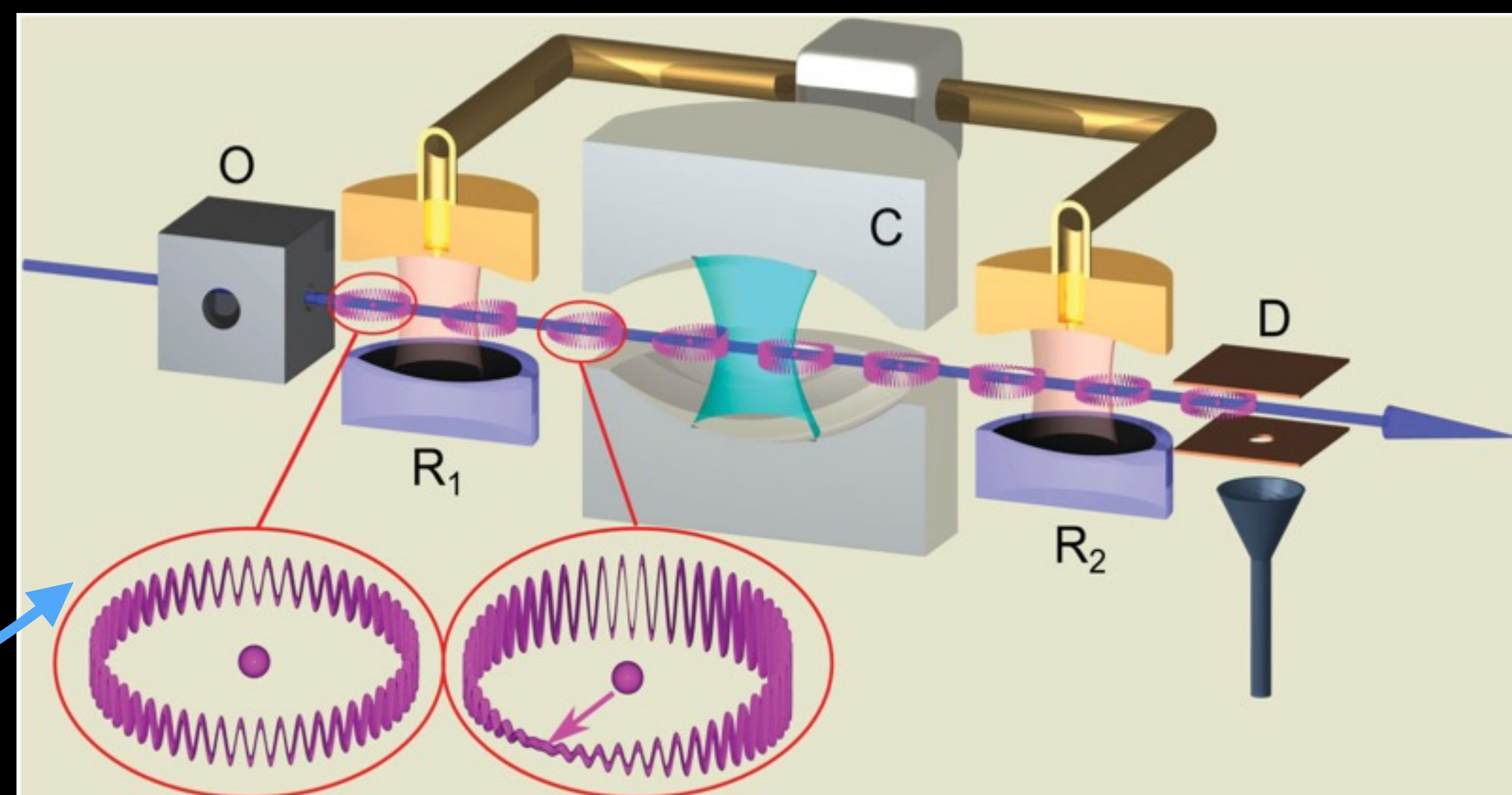
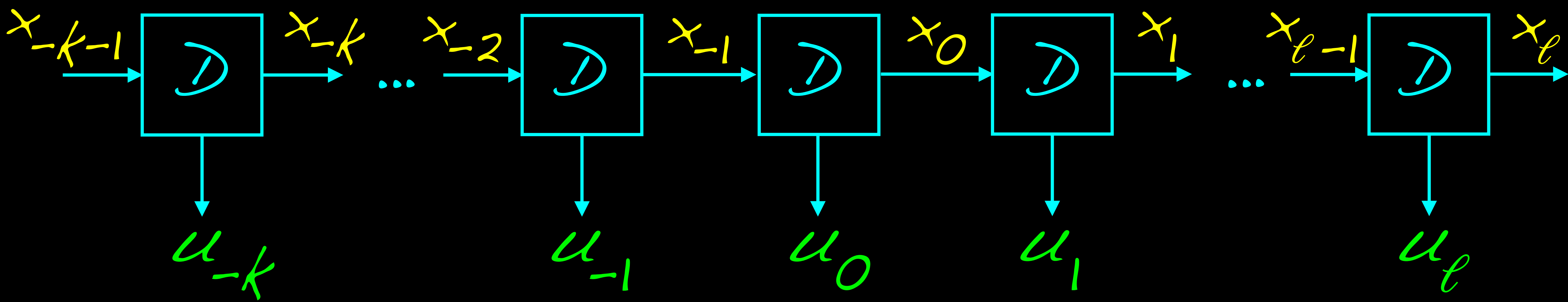


In real life (=in the laboratory):



I-c. General linear structure

The $x_t \in V$ are elements of a (real) vector space, and $\mathcal{D}$ is a collection of linear maps:



$\mathcal{D}_u : V \to V$ are linear maps, $\tau \in V$, $\pi \in V^*$, s.t.
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$\bar{\mathcal{D}}\tau = \tau$, $\pi \circ \bar{\mathcal{D}} = \pi$, as well as $\pi(\tau) = 1$.

$$P(u_1 u_2 \ldots u_\ell) = \pi \circ \mathcal{D}_{u_1} \circ \mathcal{D}_{u_2} \circ \cdots \circ \mathcal{D}_{u_\ell} \tau \qquad \text{(gu.r.)}$$

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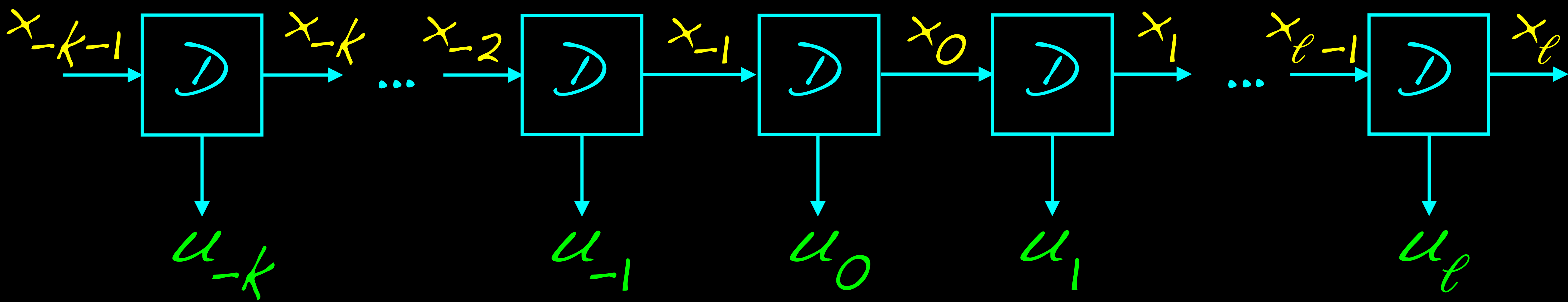

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Quasirealisation: general finitely correlated state

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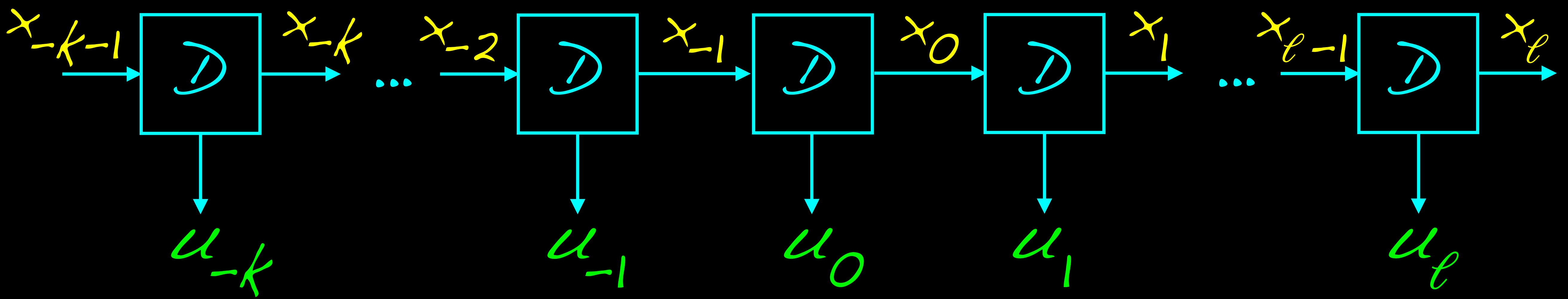

$D_u : V \to V$ are linear maps, $\tau \in V$, $\omega \in V^*$, s.t.

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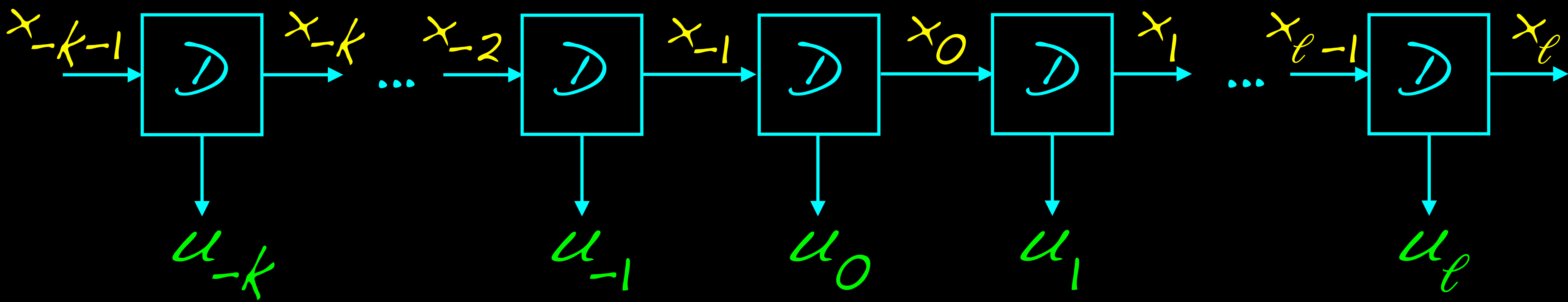

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Unlike classical and quantum case, no a priori guarantee that $P(\underline{u}) \geq 0$. In fact, checking positivity is undecidable ⚡

[Sontag, J. Comp. Syst. Sci. 11(3):375–381, 1975]

Example. $V = B(\mathbb{C}^2)_{sa} = \text{span}\{\mathbb{1}, X, Y, Z\}$ qubit with $\tau = \mathbb{1}$, $\pi = \frac{1}{2}Tr$, and the following maps:

$$D_0(A) = \frac{1}{4} |0\rangle\langle 0| A |0\rangle\langle 0|,$$
$$D_1(A) = \frac{1}{4} |1\rangle\langle 1| A |1\rangle\langle 1|,$$
$$D_x(A) = \frac{1}{4} \exp(i\alpha X) A \exp(-i\alpha X),$$
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When α/π and β/π are irrational, dynamics explores whole Bloch sphere densely. Four-dim. qu.r., but requires 2 qubits for c.p.r.!

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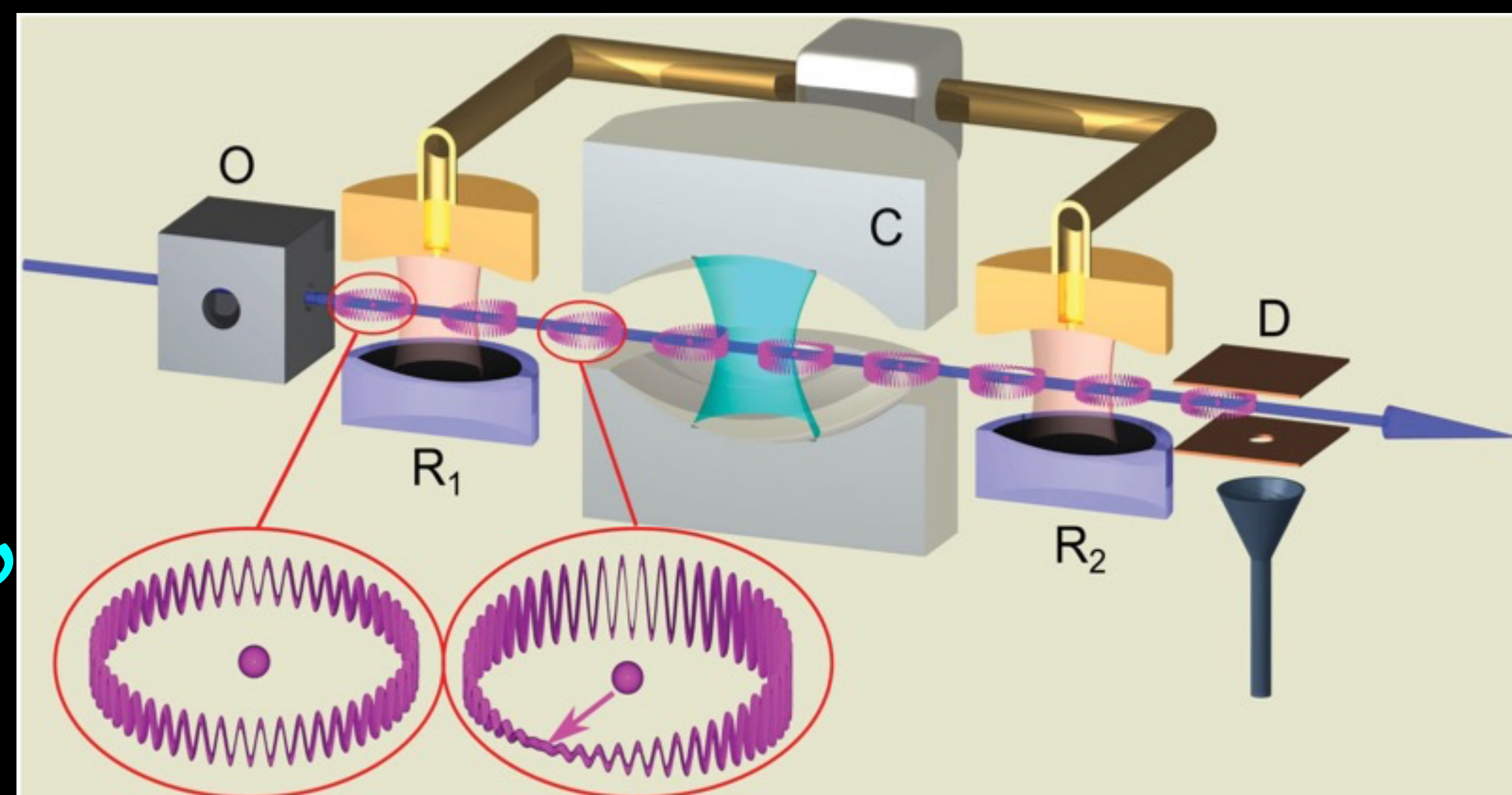
When α/π and β/π are irrational, dynamics explores whole Bloch sphere densely. Four-dim. qu.r.: HQMM with qubit memory.

Recover the internal mechanism from $P(\underline{u})$?

Quantum application: characterisation of quantum devices – state preparation, gates and measurements – from first principles. [R. Blume-Kohout et al., 1310.4492] treat system as a black box whose reaction to different interventions we can observe...



Evidently possible only up to linear equivalence, e.g. isometries.

What guarantees positivity of probability?

* $\underline{u} = u_1 u_2 \dots u_\ell \mapsto D_{\underline{u}} = D_{u_1} \circ D_{u_2} \dots \circ D_{u_\ell}$ is semigroup representation. (Notation.)

What guarantees positivity of probability?

* Classical & quantum case: positivity $P(\underline{u}) \geq 0$ enforced by the vector space order.
  Generally: Assume we have convex cones $C \subset V$ and $\tilde{C} \subset C' \subset V^*$, s.t. $\tau \in C$, $\pi \in \tilde{C}$, and the cones are preserved by the transformations, i.e. $D_u C \subset C$, $\tilde{C} D_u \subset \tilde{C}$ $\forall u$. Then $P(\underline{u}) \geq 0$.

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Dual cone $C' = \{f \in V^* : f(x) \geq 0 \ \forall x \in C\}$

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Conversely: If $P \geq 0$, then such cones exist, e.g. $C = C_{min} = \overline{\mathrm{cone}\{D_{\underline{u}}\tau : \underline{u} \in \mathbb{M}^*\}}$,

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...not unique, could for instance also take dual cone $\tilde{C} = C'$; call any such C "suitable".

Interpretation – Finite dimensional quasi-realisation "explains" time series P by the hidden mechanism of a general probabilistic theory (GPT):

- C and C' are pointed and generating cones;
- $\tau \in int(C)$ and $S := \{f \in C' : f(\tau) = 1\}$ state space;
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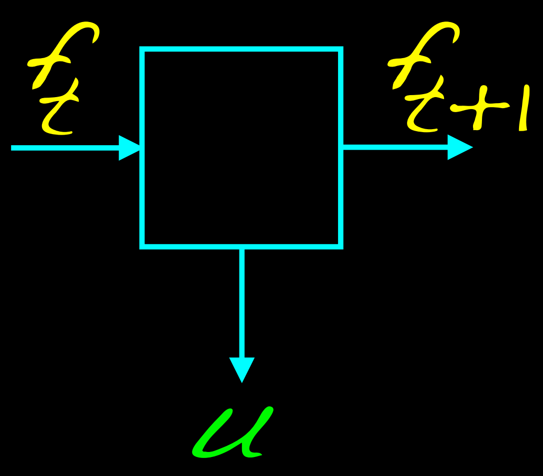

$\equiv$ { $f_t \circ D_u = \Pr\{u | f_t\} f_{t+1}$, relates current & future states, and the output u.

2. Reconstruction of V

* Consider the Hankel-type matrix $\mathcal{H} = (\mathcal{H}_{\underline{u},\underline{v}})$,
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Examples by M. Fox & H. Rubin (1968); S.W. Dharmadhikari (1970)

See later discussion

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* Conversely, if $\text{rank}\, \mathcal{H} = r < \infty$: There exists a qu.r. ("regular rep.") with $\dim V = r$, which is the minimum. Any other minimal-dim. qu.r. is <u>similar</u> to the regular one, i.e. linearly equivalent.

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Once we have that, can face the issue of finding a quantum or even classical realisation.

Related but not equivalent to the construction of the "ε-machine" [cf. Crutchfield and Santa Fe Institute].

No quantum analogue known...

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Issue: in practice, can know only a finite part of $\mathcal{H}$, i.e. some entries or more generally expectation values $\mathrm{Tr}\,\mathcal{H} M_j = \lambda_j$. (*)

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Want to find a rank-r completion of $\mathcal{H}$ with (*) and subject to constraints:

(Positivity) $\mathcal{H}_{\underline{u},\underline{v}} \geq 0$,

(Hankel) $\mathcal{H}_{\underline{u},\underline{v}} = \mathcal{H}_{\varepsilon,\underline{uv}} = \mathcal{H}_{\underline{uv},\varepsilon}$, $\mathcal{H}_{\varepsilon,\varepsilon} = 1$,

(Marginals) $\sum_{\omega} \mathcal{H}_{\underline{u},\underline{v}\omega} = \mathcal{H}_{\underline{u},\underline{v}} = \sum_{\omega} \mathcal{H}_{\omega\underline{u},\underline{v}}$

How many numbers $\lambda_j = \mathrm{Tr}\,\mathcal{H} M_j$ $(j=1,\dots,n)$ do we need to reconstruct $\mathcal{H}$, or equivalently an r-dimensional quasi-realization?

- To specify quasi-realization need less than $N := r^2|\mathbb{M}|+2r$ parameters.
- Thus expect that $n \gg N$ sufficiently random expectation values should do it...

(Work in progress)

3. Classical $\subsetneq$ quantum $\subsetneq$ GPT

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For the cone C (classical, quantum or GPT), this means intersecting it with $\mathrm{span}(C_{min})$, and factoring out $\ker(C'_{max})$.

Recall cones:

Given convex cones $C \subset V$ and $\tilde{C} \subset C' \subset V^*$, s.t. $\tau \in C$, $\pi \in C$, and the cones are preserved by the transformations, i.e. $D_u C \subset C$, $\tilde{C} D_u \subset \tilde{C}$ for all u. Then $P(\underline{u}) \geq 0$.

Conversely: If $P \geq 0$, then such cones exist, e.g. $C = C_{min} = \overline{\mathrm{cone}\{D_{\underline{u}}\tau : \underline{u} \in M^*\}}$,

$\tilde{C} = C'_{max} = \overline{\mathrm{cone}\{\pi D_{\underline{u}} : \underline{u} \in M^*\}}$.

But not unique: many cones between C_{min} and C_{max} are suitable: $C_{min} \subset C \subset C_{max}$.

(Also, of course, it has to be stable under the maps D_u!)

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A quantum realisation has the cone of semidefinite matrices; this gives rise to semidefinite representable (SDR) cones C & C' in the regular representation:

$$C = \{x=(x_1,\dots,x_d) : \exists x_{d+1},\dots x_e \sum_{i=1}^{e} x_i R_i \geq 0\},$$

for certain DxD-matrices R_i.

Example. $V = B(\mathbb{C}^2)_{sa} = \text{span}\{\mathbb{1}, X, Y, Z\}$ qubit with $\tau = \mathbb{1}$, $\pi = \frac{1}{2}Tr$, and the following maps:

$$D_0(A) = \frac{1}{4}\,|0\rangle\langle 0|\,A\,|0\rangle\langle 0|,$$
$$D_1(A) = \frac{1}{4}\,|1\rangle\langle 1|\,A\,|1\rangle\langle 1|,$$
$$D_X(A) = \frac{1}{4}\,\exp(i\alpha X)\,A\,\exp(-i\alpha X),$$
$$D_Z(A) = \frac{1}{4}\,\exp(i\beta Z)\,A\,\exp(-i\beta Z),$$
$$D_T(A) = \frac{1}{4}\,A^T.$$

When α/π and β/π are irrational, dynamics explores whole Bloch sphere densely. Four-dim. qu.r., but requires 2 qubits for c.p.r.!

In the previous example, $C_{min} = C_{max}$, hence C is unique, and it's not polyhedral: cone over Bloch sphere. Thus, this process has no (finite) classical realisation.

Polyhedral cone between C_{min} and C_{max} necessary for cl. realisation. Sufficient?

[Cf. however Fox/Rubin/Dharmadhikari!]

SDR cone between C_{min} and C_{max} necessary for existence of a quantum realisation. Sufficient? (...)

If we manage to find a quasi-realisation with $C_{min} = C_{max}$, and this cone not being SDR, this would mean that the process has no (finite) quantum realisation!

SDR cone between C_{min} and C_{max} necessary for existence of a quantum realisation. Sufficient? (...)

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Note: The processes by Fox/Rubin/Dharmadhikari/Nadkarni (1968-1970) have HQMMs in qutrits.

[M. Fanizza/J. Lumbreras/AW, arXiv:2209.11225]

SDR cone between C_{min} and C_{max} necessary for existence of a quantum realisation. Sufficient? (...)

Thm. [M. Fanizza/J. Lumbreras/AW]: $\exists$ process P with Hankel rank $\mathcal{H} = 3$ and $C_{min} = C_{max}$ transcendental, whereas SDR cones are semi-algebraic. Thus, P has no HQMM.

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Answers an open question from [Fannes/Nachtergaele/Werner, CMP 144:443-490 (1992)] :-)

Example: P has three symbols, 0, 1, 2.
We give directly its quasi-realisation:
$V=\mathbb{R}^3$; let $a>1>b>0$ such that $\ln a$ and $\ln b$ are linearly independent over the rationals.

$$D_1 = \begin{bmatrix} a & 0 & 0 \\ 0 & 1 & 0 \\ 0 & \ln a & 1 \end{bmatrix}, \quad D_2 = \begin{bmatrix} b & 0 & 0 \\ 0 & 1 & 0 \\ 0 & \ln b & 1 \end{bmatrix},$$

$$D_0 = m_0 \mu_0^T, \text{ with } m_0 = \begin{bmatrix} m_{01} \\ m_{02} \\ m_{03} \end{bmatrix},$$

$$\mu_0^T = [\mu_{01} \ \mu_{02} \ \mu_{03}]$$

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$$D_1^s D_2^t = \begin{bmatrix} a^s b^t & 0 & 0 \\ 0 & 1 & 0 \\ 0 & s(\ln a)+t(\ln b) & 1 \end{bmatrix} \text{ for } s,t \in \mathbb{N}$$

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$$D_1^s D_2^t = \begin{bmatrix} e^x & 0 & 0 \\ 0 & 1 & 0 \\ 0 & x & 1 \end{bmatrix}, \text{ with } x \in \mathbb{R} \text{ dense!}$$

Example (cont'd): M_0 is a "reset" operation, which allows us to write

$$C'_{max} = \text{cone}\{[\mu_{01}e^x \ \ \mu_{02}+\mu_{03}x \ \ \mu_{03}] : x\in\mathbb{R}\}$$

$$C_{min} = \text{cone}\{[m_{01}e^x \ \ m_{03} \ \ m_{02}+m_{03}x]^T : x\in\mathbb{R}\}$$

Fact: C_{max} is of the same form as C_{min}, only with different parameters. One can choose D_0 such that $C_{min}=C_{max}=C$.

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In that case, a suitable positive linear combination of D_0, D_1, D_2 has right fixed point τ in $\mathrm{int}(C)$, and left fixed point π in $\mathrm{int}(C')$. This is the sought-after qu.r. (...)

Example gives rise to the exponential cone

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More examples from power cone $(0 \leq t \leq 1)$

$$K_t = \{(x,y,z) : x^t + y^t \geq |z|,\ x,y \geq 0, z \in \mathbb{R}\},$$

which is transcendental iff t is irrational.

As before we can design a reset map and two invertible maps, which latter act densely transitive on the cone's extremal rays. And we can engineer $C_{min} = C_{max}$, too.

4. Further thoughts

Extend to genuinely quantum case, i.e. a chain of non-commutative spin C^*-algebras:

- Have a generalisation of regular (minimum dim.) representation for finitely corr. states
- Rather than a vector space order on V and positive elements and maps, necessary and sufficient structure is an operator system, i.e. consistent orders on $V \otimes M_n$, and maps are completely positive...

[Fannes/Nachtergaele/Werner, CMP 144:443-490 (1992)]

4. Further thoughts

Finitely correlated state on a chain of non-commutative spin C^*-algebras:

- In fact, the finitely correlated state itself gives us two extreme o.s., where the cones $(V \otimes M_n)_+$ are either all as small or all as large as they can be.
- Exponential and power cones have matrix generalisations; perhaps suitable for new variational classes of finitely corr. states?

[Fanizza et al., in preparation]

4. Questions, questions, questions

- Low-rank completion of the Hankel matrix with noisy data?
- How to find a quantum model just from the regular representation (assuming one exists)?
- Can these exponential and power cones be useful? Note that dual cone is of the same kind, so perhaps good for convex optimisation. Interesting class of GPTs?
- CP maps for matrix power & exp. cones?

=Additional material=


Ogni scarrafon' è
bell' a mamma suja

5. Removing redundancy: quotients

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Null space; $C \cap K = 0$, so we may factor out K...

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$V_0 := W/K$,

$C_0 := (C \cap W)/K = \{w + K : w \in C \cap W\}$,

$\tau_0 := \tau + K$, $\pi_0 := \pi/K$, $D_u^0 := D_u/K$; well-defined because of $\pi(K) = 0$, $D_u W \subset W$, $D_u K \subset K$.

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Always a minimal-dim. qu.r., hence is isomorphic to regular, and cone C_0 is suitable.

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Classical model, i.e. $V = \mathbb{R}^d$, $C = \mathbb{R}^d_{\geq 0}$, $\tau = (1, \dots, 1)^\top$,

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C_0 is then a polyhedral cone and every such cone arises in the above way (Fourier-Motzkin elemination). Guaranteed:

$d \leq$ #extremal rays of C, sometimes best.

5'. Quotient of a quantum model

Quantum model, i.e. $V = B(\mathcal{H})_{sa}$, $C = B(\mathcal{H})_{\geq 0}$, $\tau = \mathbb{1}$, $\pi = \omega$ quantum state, D_u are cp maps.

Once constructed $K \cap W \subset W \subset V$: $C \cap W$ is an operator system, $C_0 = (C \cap W)/K$ a quotient operator system; the D_u^0 preserve C, in fact cp maps in the operator system sense.

[Farenick/Paulsen, Math. Scand. 111:210-243, 2012]

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[Farenick/Paulsen, Math. Scand. 111:210-243, 2012]

Membership in the cone is an SDP: semi-definite condition of a finite-size matrix with existential real variables.

SDR operator systems:

$\mathbb{1} \in \mathcal{W} = \mathrm{span}\{\mathcal{D}_{\underline{u}}\mathbb{1} : \underline{u} \in \mathbb{M}^*\} = \mathcal{B}(\mathcal{H})_{sa}$,

$K = \{\omega \circ \mathcal{D}_{\underline{u}} : \underline{u} \in \mathbb{M}^*\}^{\perp} \subset \mathcal{B}(\mathcal{H})_{sa}$.

Vector space and positive cone:

$V_0 := \mathcal{W}/K$,

$C_0 := (\mathcal{B}(\mathcal{H})_{\geq 0} \cap \mathcal{W})/K = \{w + K : w \in \mathcal{B}(\mathcal{H})_{\geq 0} \cap \mathcal{W}\}$.

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Operator system lifts this to $V_0 \otimes B(\mathbb{C}^n)_{sa}$:

$C_n := (B(\mathcal{H} \otimes \mathbb{C}^n)_{\geq 0} \cap \mathcal{W} \otimes B(\mathbb{C}^n)_{sa})/K \otimes \mathbb{1}$

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CP maps: $(\mathcal{D}_u \otimes id)C_n \subset C_n$ for all u and n.

[Farenick/Paulsen, Math. Scand. 111:210-243, 2012]

But the $\mathcal{D}_{\mathcal{U}}^{o}$ remember more than just being cp in the operator system. Indeed,

$$\mathcal{D}_{\mathcal{U}}^{o} \in \mathscr{P} := \{\Lambda/K : \Lambda \text{ cp on } B(\mathcal{H}), \quad \Lambda(\mathcal{W}) \subset \mathcal{W},\ \Lambda(K) \subset K\} \subset End(V_0),$$

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$\mathcal{P}=\mathcal{P}(\mathcal{W},K) \subset CP(V_0)$, and in general the inclusion is strict!

[Equality by Arveson's extension theorem for $K=0$ or $\mathcal{W}=B(\mathcal{H})_{sa}$]

6. Reconstructing the vector order?

Task: Find a suitable cone C for the qu.r. $(V, \tau, \pi, \mathcal{D}_u)$, ideally a "nice" one...

Necessarily, $C_{min} \subset C \subset C_{max}$, with (recall)

$$C_{min} = \overline{\text{cone}\{\mathcal{D}_{\underline{u}}\tau : \underline{u} \in \mathbb{M}^*\}},$$

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Can we choose C polyhedral or SDR?

Difficulty of course that C has to be preserved by the D_u; note that C_{min} & C_{max} satisfy this automatically.

6. Reconstructing the vector order?

Instructive special case: $C = C_{min} = C_{max}$, ruling out a classical model if that is not a polyhedral cone. [Cf. example, where this happens with C=cone over a Bloch sphere.]

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Instructive special case: $C = C_{min} = C_{max}$, ruling out a classical model if that is not a polyhedral cone. [Cf. example, where this happens with C=cone over a Bloch sphere. And the other example, where C is unique and not SDR, in fact transcendental; provides a process generated by a finite GPT, but w/o quantum realisation.]