On the Reversal of the (Statistical) Laws of Nature: Schrödinger, Kolmogorov and Landauer. Some elements for the history of an idea.

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based on joint work with

Raphaël Chétrite and Kay Schwieger.

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Schrödinger in Berlin Moore, *Schrödinger: Life and Thought*, (1989)

- 1927 Chair of theoretical physics at Friedrich Wilhelms Universität.
- 1929: unanimously elected to the Prussian Academy of Sciences.
- At the age of 42 was the youngest member.
- Academy founded by Gottfried Wilhelm Leibniz in 1700.
- Notable members Einstein, Planck, Laue, and Nernst.
- Friendship with Einstein.
- January 30, 1933, Hitler Chancellor of Germany.
- July 1933 Anny and Erwin Schrödinger leave Berlin for good on a grey cabriolet B.M.W.

"On the Reversal of the Laws of Nature" arXiv:2105.12617

144 Sitzung der physikalisch-mathematischen Klasse vom 12. März 1931

Über die Umkehrung der Naturgesetze.

Von E. Schrödinger.

Einleitung. Wenn für ein diffundierendes oder in Brownscher Bewegung begriffenes Teilchen die Aufenthaltswahrscheinlichkeit im Abszissenbereich $(x; x+dx)$ zur Zeit t_0

$$w(x, t_0)\,dx$$

gegeben ist,

$$w(x, t_0) = w_0(x),$$

so ist sie für $t > t_0$ diejenige Lösung $w(x, t)$ der Diffusionsgleichung

$$D\frac{\partial^2 w}{\partial x^2} = \frac{\partial w}{\partial t}, \tag{1}$$

welche für $t = t_0$ der vorgegebenen Funktion $w_0(x)$ gleich wird. — Über

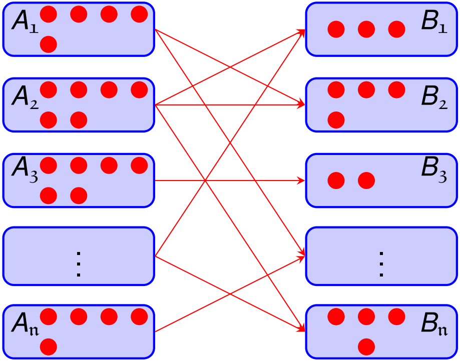
Particle Migration Model

- Two sets of $\mathfrak{n}$ boxes

$$\{A_i\}_{i=1}^{\mathfrak{n}} \quad \& \quad \{B_i\}_{i=1}^{\mathfrak{n}}$$

- N particles initially randomly located in $\{A_i\}_{i=1}^{\mathfrak{n}}$
- Each *migration* is an independent event

$$g_{ij} = \Pr(\text{be in } A_i \text{ then be in } B_j)$$



Migration as a random process

- Random migration $\Leftrightarrow$ Matrix valued random variable $\mathscr{C} = \{\mathcal{c}_{ij}\}_{ij=1}^{\mathfrak{n}}$ such that $\sum_{i,j=1}^{\mathfrak{n}} \mathcal{c}_{ij} = N$
- Realization of the migration $\Leftrightarrow$ Realization of the random variable: $C = \{c_{ij}\}_{ij=1}^{\mathfrak{n}}$ such that $\sum_{i,j=1}^{\mathfrak{n}} c_{ij} = N$

Meaning of the random variable

$$c_{ij} = \#(\text{particles first in } A_i \text{ and then migrating to } B_j)$$

Marginal particle distributions and related "marginal" random variables

$$a_i = \sum_{j=1}^{\mathfrak{n}} c_{ij} = \#(\text{particles in } A_i) \quad \Rightarrow \quad \tilde{\mathscr{C}}_A = \sum_{j=1}^{\mathfrak{n}} \mathcal{c}_{ij}$$

$$b_j = \sum_{j=1}^{\mathfrak{n}} c_{ij} = \#(\text{particles in } B_j) \quad \Rightarrow \quad \tilde{\mathscr{C}}_B = \sum_{i=1}^{\mathfrak{n}} \mathcal{c}_{ij}$$

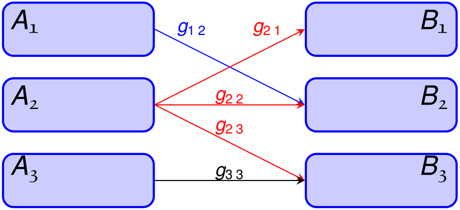
The "standard" probabilistic approach

- Assign initial marginal

$$\tilde{\mathscr{C}}_A = \boldsymbol{a}$$

- Assign the joint probabilities

$$g_{i\,j} = \Pr(\text{be in } A_i \text{ then be in } B_j)$$



Probability of a migration C given an initial distribution $\boldsymbol{a}$

$$\Pr(\mathscr{C} = C \ | \widetilde{\mathscr{C}} = \boldsymbol{a}) = \left(\prod_{i=1}^{n} a_i!\right) \prod_{i\,j=1}^{n} \frac{1}{c_{i\,j}!} \left(\frac{g_{i\,j}}{\sum_{j=1}^{n} g_{i\,j}}\right)^{c_{i\,j}}$$

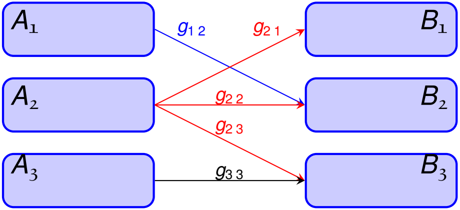
Schrödinger's problem

H.1 Assign initial marginal

$$\tilde{\mathscr{C}}_A = \boldsymbol{a}$$

H.2 Assign the final marginal

$$\tilde{\mathscr{C}}_B = \boldsymbol{b}$$



Reversibility

- Is it possible to construct a **new** migration process with probability

$$k_{i\,j} \text{ "close" to } g_{i\,j}$$

  such that (**H.1**), (**H.2**) always hold?
- If yes: what if the marginals exchange roles (i.e. the process is reversed)

Schrödinger's "large deviation" approach

- suppose $N \gg 1$
- rescale and define empirical probability distributions

$$a_i = N\, w_{\rm o}(i) \qquad \& \qquad b_i = N\, w_{1}(i)$$
$$c_{i\,j} = N\, k_{i\,j}$$

- Introduce transition probabilities

$$g_{i\,j} = g(j|i)\, w_{\rm o}(i) \qquad \text{reference process}$$
$$k_{i\,j} = k(j|i)\, w_{\rm o}(i) \qquad \text{empirical process}$$

Stirling's formula

$$\Pr(\mathscr{C} = C \,|\, \tilde{\mathscr{C}} = \boldsymbol{a}) \sim \exp\left(-N \sum_{i\,j=1}^{\mathfrak{n}} k(j|i)\, w_{\rm o}(i) \ln \frac{k(j|i)}{g(j|i)} \right)$$

How close are two probability distributions?

Kullback–Leibler divergence
Kullback and Leibler, *Annals of Mathematical Statistics*, (1951)

$$\mathrm{D}_{KL}(\mathrm{K}\|\mathrm{G}) = \sum_{i\,j=1}^{\mathfrak{n}} k(j|i)\, w_{\circ}(i) \ln \frac{k(j|i)}{g(j|i)}$$

The smallest D_{KL} the closest $\mathrm{K} = \{k(j|i)\}_{i\,j=1}^{\mathfrak{n}}$ to $\mathrm{G} = \{g(j|i)\}_{i\,j=1}^{\mathfrak{n}}$

- In large deviation theory Kullback–Leibler minimization is used to determine the most likely configuration **San1957**, **San1957**, (**San1957**).
- Schrödinger uses D_{KL}-minimization as tool to construct a new conditional probability "close" to the reference process but interpolating between assigned marginals.

$$w_{1}(i) = \sum_{j=1}^{\mathfrak{n}} k(i|j) w_{\circ}(j)$$

Schrödingers' optimal control problem

Minimize with respect to the $k(j|i)$'s the Kullback–Leibler divergence

$$\mathrm{D}_{KL}(\mathrm{K}\|\mathrm{G}) = \sum_{i\,j=1}^{n} k(j|i)\, w_{0}(i) \ln \frac{k(j|i)}{g(j|i)}$$

Under the constraints

- $w_{1}(i) = \sum_{j=1}^{n} k(i|j) w_{0}(j)$
- $\sum_{i=1}^{n} k(i|j) = 1$

Warning: change of paradigm

The purpose of the large deviation calculation is to justify the use of the Kullback–Leibler divergence (still to be discovered in 1931!) to construct a diffusion process between fixed end states.

Schrödingers' optimal mass transport

The optimum problem is equivalent to: find φ_1, φ_0 such that

$$w_1(i) = \varphi_1(i) \sum_{j=1}^{n} g(i|j)\, \varphi_0(j)$$

$$w_0(j) = \varphi_0(j) \sum_{i=1}^{n} \varphi_1(i)\, g(i|j)$$

"Born's law" for the interpolating density

Additional hypothesis:

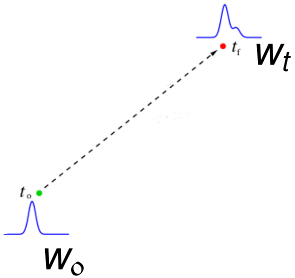
there exists continuously in $t \in [0, 1]$ a $p_t(i|j)$ such that

$$p_0(i|j) = \delta_{ij}$$
$$p_1(i|j) = g(i|j)$$

Born law: $w_t(i) = \bar{h}_t(i)\, h_t(i)$

$$\bar{h}_t(i) = \sum_{j=1}^{n} p_t(i|j)\, \varphi_0(j)$$

$$h_t(i) = \sum_{i=1}^{n} \varphi_1(j)\, p_t(j|i)$$



Kolmogorov 1936: **Kol1936**, **Kol1936**, (**Kol1936**)

Zur Theorie der Markoffschen Ketten.

Von

A. Kolmogoroff in Moskau.

Die nachfolgenden Betrachtungen scheinen mir, trotz ihrer Einfachheit, neu und nicht ohne Interesse für gewisse physikalische Anwendungen zu sein, insbesondere für die Analyse der Umkehrbarkeit der statistischen Naturgesetze, welche Herr Schrödinger im Falle eines speziellen Beispiels durchgeführt hat[1]). In der ganzen weiteren Darstellung ist es gleichgültig, welche der beiden folgenden Voraussetzungen über die in Betracht kommenden Werte der Zeitkoordinate t gemacht wird: entweder durchläuft t alle reellen Werte, oder man beschränkt sich auf die Heranziehung der ganzzahligen Werte von t. Der klassischen Auffassung Markoffscher Ketten entspricht die zweite Möglichkeit.

"*The following considerations seem to me, in spite of their simplicity, to be new and not without interest for certain physical applications, in particular for the analysis of the reversibility of the statistical laws of Nature, which Mr. Schrödinger carried out in the case of a special example.*"

Time reversal of Markov processes

Assumptions: Markov process for which we know

- the transition probability density $\mathcal{g}_{t\,s}$ for any $s \leq t \in [t_{\mathrm{o}}\,, t_{\mathrm{f}}]$;
- a particular solution p_t **strictly positive** for all $t \in [t_{\mathrm{o}}\,, t_{\mathrm{f}}]$.

Joint probability density of the Markov process at any times s and t

$$\mathcal{c}_{t\,s}(\boldsymbol{x}, \boldsymbol{y}) = \mathcal{g}_{t\,s}(\boldsymbol{x}|\boldsymbol{y})p_s(\boldsymbol{y})$$

Reversed transition probability associated to the density g_t

$$\mathcal{g}^{(r)}_{s\,t}(\boldsymbol{y}|\boldsymbol{x}) = \frac{\mathcal{c}_{t\,s}(\boldsymbol{x}, \boldsymbol{y})}{p_t(\boldsymbol{x})} = \frac{\mathcal{g}_{t\,s}(\boldsymbol{x}|\boldsymbol{y})p_s(\boldsymbol{y})}{p_t(\boldsymbol{x})}$$

or equivalently

$$p_t(\boldsymbol{x})\,\mathcal{g}^{(r)}_{s\,t}(\boldsymbol{y}|\boldsymbol{x}) = \mathcal{g}_{t\,s}(\boldsymbol{x}|\boldsymbol{y})p_s(\boldsymbol{y})$$

Consequences for Schrödinger's mass transport

- In general: well defined relations under exchange

$$w_0 \longleftrightarrow w_1$$

- In the presence of detailed balance (reversal wrt stationary measure $p_\star$)

$$p_\star(\boldsymbol{x})\, g_{t-s}(\boldsymbol{y}|\boldsymbol{x}) = g_{t-s}(\boldsymbol{x}|\boldsymbol{y})\, p_\star(\boldsymbol{y})$$

the relations simply become

$$(\varphi_0, \varphi_1) \to \left(\varphi_1\, p_\star, \frac{\varphi_0}{p_\star}\right)$$

$$(h_t, \bar{h}_t) \longrightarrow \left(\bar{h}_{t_0+t_f-t}\, p_\star, \frac{h_{t_0+t_f-t}}{p_\star}\right)$$

$$w_t \longrightarrow w_{t_0+t_f-t}$$

Landauer 1961 **Lan1961**, **Lan1961**, (**Lan1961**)

R. Landauer

Irreversibility and Heat Generation in the Computing Process

Abstract: It is argued that computing machines inevitably involve devices which perform logical functions that do not have a single-valued inverse. This logical irreversibility is associated with physical irreversibility and requires a minimal heat generation, per machine cycle, typically of the order of kT for each irreversible function. This dissipation serves the purpose of standardizing signals and making them independent of their exact logical history. Two simple, but representative, models of bistable devices are subjected to a more detailed analysis of switching kinetics to yield the relationship between speed and energy dissipation, and to estimate the effects of errors induced by thermal fluctuations.

Landauer's principle: information is physical.

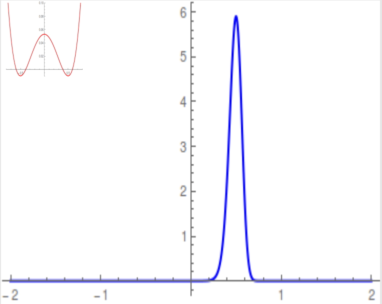
Logical irreversible computing operations

$\Leftrightarrow$

irreversible thermodynamic transitions.

Bit erasure

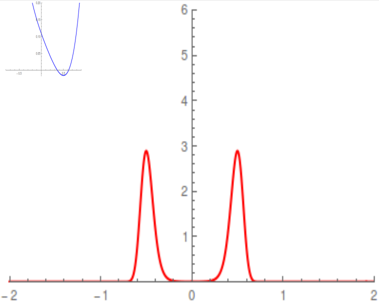
Turn one well into a double well



Initial state

Controlled

Markovian dynamics



Final state

Today: expermental verifications of Landauer's principle

LETTER

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Experimental verification of Landauer's principle linking information and thermodynamics

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In 1961, Rolf Landauer argued that the erasure of information is a dissipative process[1]. A minimal quantity of heat, proportional to the thermal energy and called the Landauer bound, is necessarily produced when a classical bit of information is deleted. A direct consequence of this logically irreversible transformation is that the entropy of the environment increases by a finite amount. Despite its fundamental importance for information theory and computer science[2–5], the erasure principle has not been verified experimentally so far, the main obstacle being the difficulty of doing single-particle experiments in the low-dissipation regime. Here we experimentally show the existence of the Landauer bound in a generic model of a one-bit memory. Using a system of a single colloidal particle trapped in a modulated double-well potential, we establish that the mean dissipated heat saturates at the Landauer bound in the limit of long erasure cycles. This result demonstrates the intimate link between information theory and thermodynamics. It further highlights the ultimate physical limit of irreversible computation.

fundamental physical limit of irreversible computation. However, its validity has been repeatedly questioned and its usefulness criticized[17–22]. From a technological perspective, energy dissipation per logic operation in present-day silicon-based digital circuits is about a factor of 1,000 greater than the ultimate Landauer limit, but is predicted to quickly attain it within the next couple of decades[23,24]. Moreover, thermodynamic quantities on the scale of the thermal energy kT have been measured in mesoscopic systems such as colloidal particles in driven harmonic[25] and non-harmonic optical traps[26].

To verify the erasure principle experimentally, we consider, following the original work of Landauer[1], an overdamped colloidal particle in a double-well potential as a generic model of a one-bit memory. For this, we use a custom-built vertical optical tweezer that traps a silica bead (2 μm in diameter) at the focus of a laser beam[27,28]. We create the double-well potential by focusing the laser alternately at two different positions with a high switching rate. The exact form of the potential is determined by the laser intensity and by the distance between the two focal points

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Experimental realization of a Szilard engine with a single electron

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The most succinct manifestation of the second law of thermodynamics is the limitation imposed by the Landauer principle on the amount of heat a Maxwell demon (MD) can convert into free energy per single bit of information obtained in a measurement. We propose and realize an electronic MD based on a single-electron box operated as a Szilard engine, where k_BT ln 2 of heat is extracted from the reservoir at temperature T per one bit of created information. The information is encoded in the position of an extra electron in the box.

Our experimental realization of the SE cycle is shown in Fig. 1*C*. Its main element is the single-electron box (SEB) (14–16), which consists of two small metallic islands connected by a tunnel junction. The SEB is maintained at the dilution-refrigerator temperatures in the 0.1-K range. Physically, there are two main differences between the SEB and the original single-molecule SE. The electrodes of the box contain electron gas of a large number of electrons, and not just one particle. Consequently, what is being manipulated in the engine operation is not this

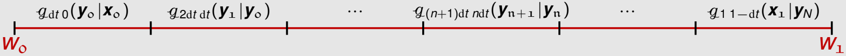
Mathematically

Optimal control of a stochastic dynamics in finite time between pre-assigned probability distributions at the end of the control time horizon.

Gawędzki, "Fluctuation Relations in Stochastic Thermodynamics", *arXiv:1308.1518*, (2013)

Optimal control of microscopic dynamics

Microscopic dynamics



- Kullback–Leibler divergence in pathspace: depends upon all conditional probabilities of two Markov processes on arbitrary $\mathrm{d}t \downarrow$ partitions of the control horizon.
- specified by microscopic dynamics (e.g. SDEs)

Optimization

Schrödinger diffusion

Kullback–Leibler divergence of the path measure of the controlled from the reference process.

Stochastic thermodynamics

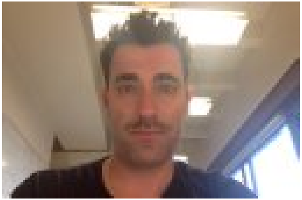
Kullback–Leibler divergence of the path measure of a forward process from a process defined by a time reversal operation.

Conclusions

Schrödinger diffusion in statistical physics and engineering

- Shows how to steer a controlled Markov process between pre-assigned end states, by keeping it as close as possible to a reference Markov process for which only one of the end states can be assigned.
- In a micro-scale level description of the dynamics, (Langevin-Smoluchowski limit) Schrödinger's diffusion specifies "viscosity" solutions of the optimal evolution between assigned states at minimum dissipation: Landauer's principle.
- More generally: optimal control problems of thermodynamic transitions between given states correspond to a change of the cost function in Schrödinger's original probem.

THANKS, Raphaël & Kay



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