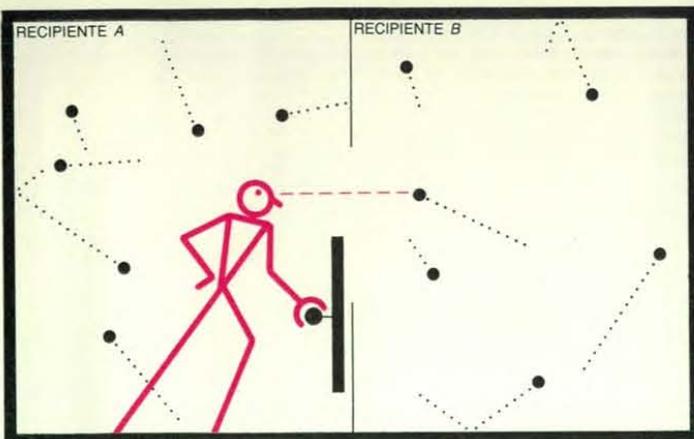# la strana termodinamica del mondo dei quanti

massimo palma
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NEST - CNR

sommario

- il diavolo di Maxwell, entropia ed informazione

- entanglement e sistemi multipartiti

- tipicalità

- lavoro, calore, cicli termodinamici

il diavoletto di Maxwell

Il diavoletto di Maxwell, descritto nel 1871 da James Clerk Maxwell, sembra in grado di violare il secondo principio della termodinamica. Il diavoletto aziona una porticina su un setto posto fra due recipienti che contengono gas alla stessa temperatura e pressione. Egli osserva le molecole che si avvicinano al foro e apre o chiude la porticina lasciando passare le molecole più veloci dal recipiente A a quello B, ma non viceversa, e quelle più lente solo da B ad A. Il recipiente B si riscalda, mentre l'altro si raffredda. Per il secondo principio occorre lavoro per produrre una differenza di temperatura, ma il lavoro per azionare la porta può essere reso piccolo a piacere.
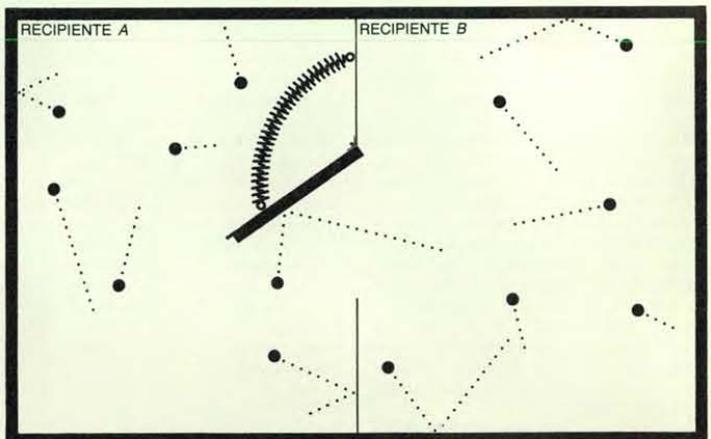
Con una porticina a molla si può realizzare una versione automatica del diavoletto di Maxwell che produce una differenza di pressione anziché di temperatura. Fra due recipienti contenenti inizialmente gas alla stessa pressione e temperatura vi è un foro munito di una porticina a molla. La porticina si apre in una sola direzione, per lasciare passare le molecole dal recipiente B al recipiente A, ma non viceversa. Si può pensare che, alla fine, le molecole si accumulino in A a spese di B, producendo una differenza di pressione. Ma, in pratica, questo non può avvenire. La porticina, riscaldata dagli urti con le molecole, prende ad aprirsi e a chiudersi casualmente per agitazione termica. Quando è aperta non può fungere da valvola a flusso unidirezionale e quando si chiude può spingere una molecola da A a B. Il secondo processo avviene altrettanto frequentemente di quello nel quale una molecola di B spinge la porta per passare in A.
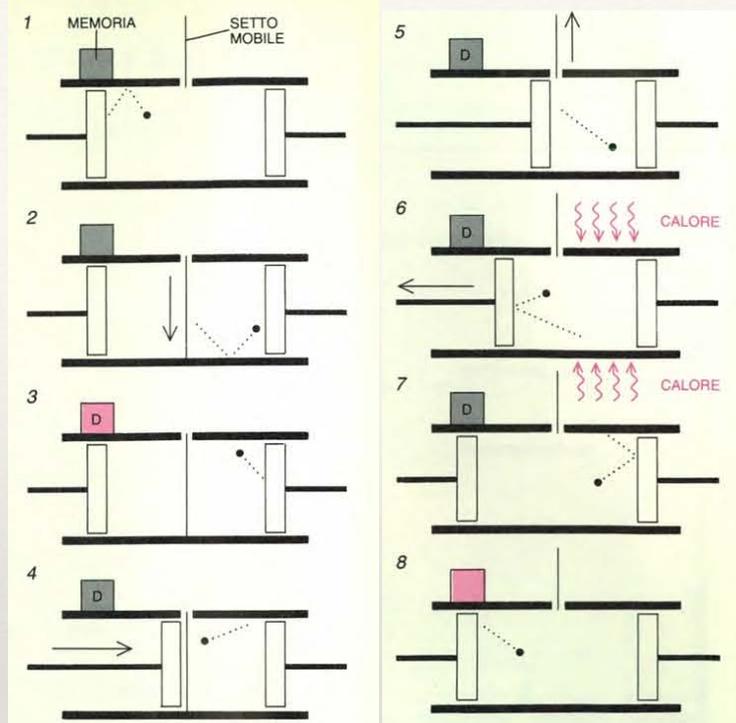
La macchina di Szilard

per non violare il secondo principio e' necessario che nel ciclo venga dissipata un energia pari a KTln2
Secondo il principio di Landauer questa energia viene dissipata quando viene cancellata la memoria

La macchina di Szilard, descritta da Leo Szilard nel 1929, sembra poter convertire il calore dell'ambiente in lavoro, violando il secondo principio. La macchina (1) è costituita da un cilindro con le estremità chiuse da pistoni; è munita di un setto mobile e di apparecchiature per osservare il contenuto del cilindro e memorizzare le osservazioni. Il cilindro contiene una sola molecola. All'inizio del ciclo (2) si abbassa il setto, intrappolando la molecola in una metà del cilindro. Il sistema di osservazione determina e memorizza la posizione della molecola (3) e il pistone dalla parte opposta viene spinto fino a toccare il setto (4). Il pistone viene spostato senza compiere lavoro, dato che si muove nel vuoto. Poi il setto viene ritirato (5) e la molecola urta il pistone (il gas monomolecolare si «espande»), spingendolo indietro (6). L'energia spesa dalla molecola nel compiere lavoro sul pistone è compensata dal calore sottratto all'ambiente. Quando il pistone è tornato nella posizione originale (7), la memoria viene cancellata (8) e il ciclo può ricominciare.

entangled states, entropy and typicality

$$\frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\uparrow\rangle + |\downarrow\rangle|\downarrow\rangle\right)$$
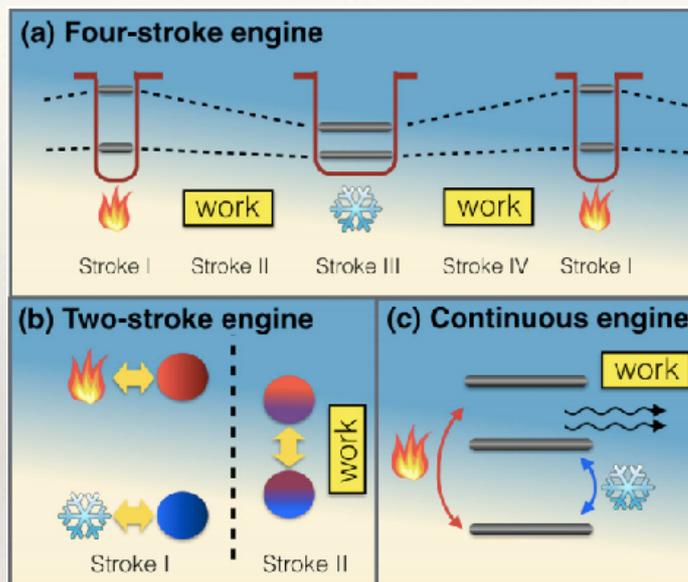
lo stato complessivo e' puro ma gli stati ridotti sono misti

gli stati tipici di un sistema multipartito sono fortemente entangled
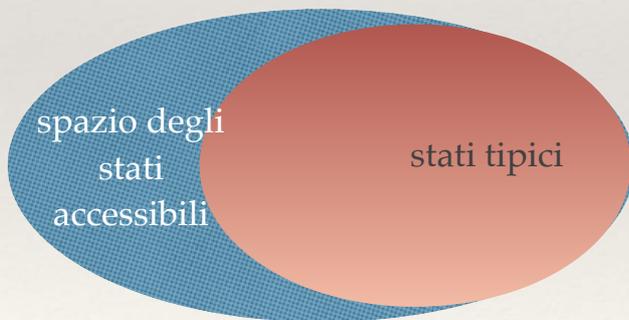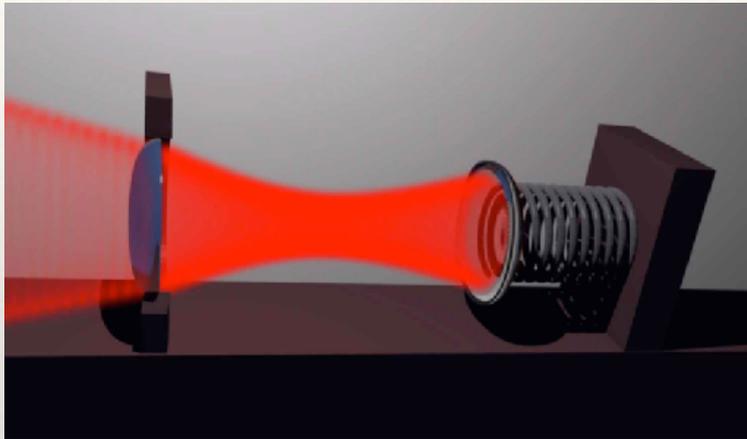
è possibile ottenere uno stato "termico" come parte di uno stato puro di uno spazio di hilbert "grande"

spazio degli stati accessibili

stati tipici

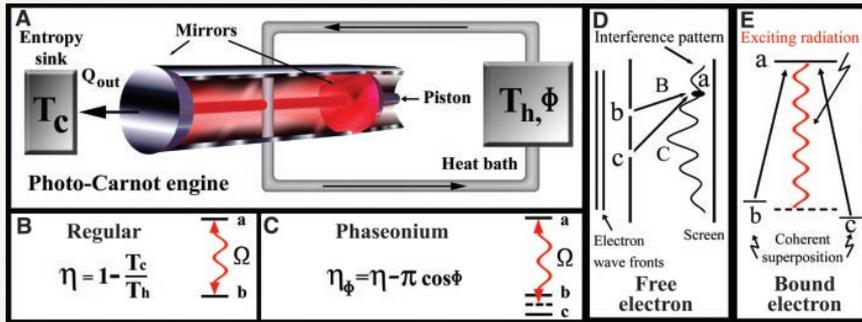# macchine termodinamiche quantistiche

quantum optomechanics

Fig. 1. (**A**) Photo-Carnot engine in which radiation pressure from a thermally excited single-mode field drives a piston. Atoms flow through the engine and keep the field at a constant temperature T_{rad} for the isothermal $1 \rightarrow 2$ portion of the Carnot cycle (Fig. 2). Upon exiting the engine, the bath atoms are cooler than when they entered and are reheated by interactions with the hohlraum at T_h and "stored" in preparation for the next cycle. The combination of reheating and storing is depicted in (A) as the heat reservoir. A cold reservoir at T_c provides the entropy sink. (**B**) Two-level atoms in a regular thermal distribution, determined by temperature T_h, heat the driving radiation to $T_{rad} = T_h$ such that the regular operating efficiency is given by η. (**C**) When the field is heated, however, by a phaseonium in which the ground state doublet has a small amount of coherence and the populations of levels a, b, and c, are thermally distributed, the field temperature is $T_{rad} > T_h$, and the operating efficiency is given by η_ϕ, where π can be read off from Eq. 7. (**D**) A free electron propagates coherently from holes b and c with amplitudes B and C to point a on screen. The probability of the electron landing at point a shows the characteristic pattern of interference between (partially) coherent waves. (**E**) A bound atomic electron is excited by the radiation field from a coherent superposition of levels b and c with amplitudes B and C to level a. The probability of exciting the electron to level a displays the same kind of interference behavior as in the case of free electrons; i.e., as we change the relative phase between levels b and c, by, for example, changing the phase of the microwave field which prepares the coherence, the probability of exciting the atom varies sinusoidally, as indicated in Eq. 4.
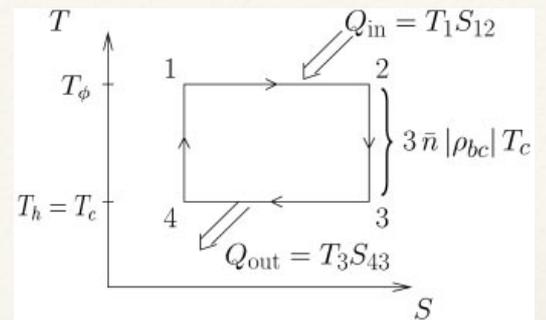
Fig. 2. Temperature-entropy diagram for Carnot cycle engine. In the present QHE, Q_{in} is provided by the hot atoms. When $T_h = T_c$, the photo-Carnot engine can still produce useful work if the coherent three-level heat bath atoms (Fig. 1C) are "phased" such that $\phi = \pi$.

Extracting Work from a Single Heat Bath via Vanishing Quantum Coherence

Marlan O. Scully,[1,2] M. Suhail Zubairy,[1,3] Girish S. Agarwal,[1,4] Herbert Walther[2]

ion traps
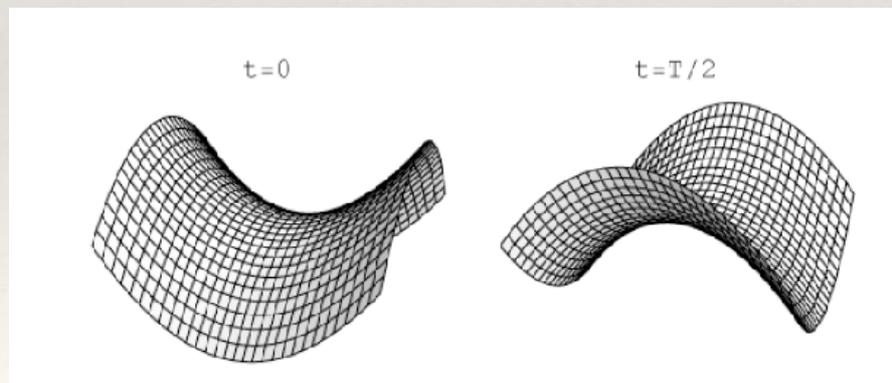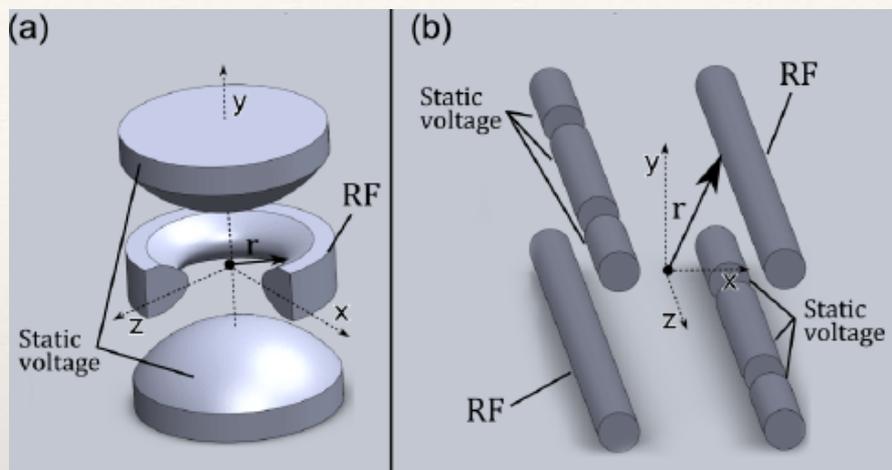
quantum Otto cycle
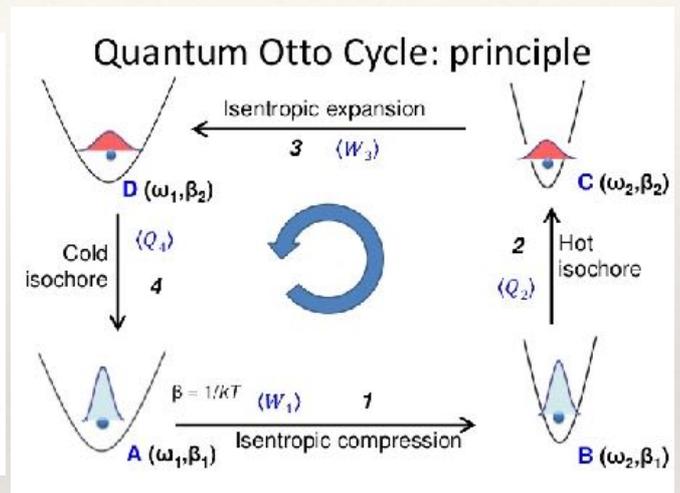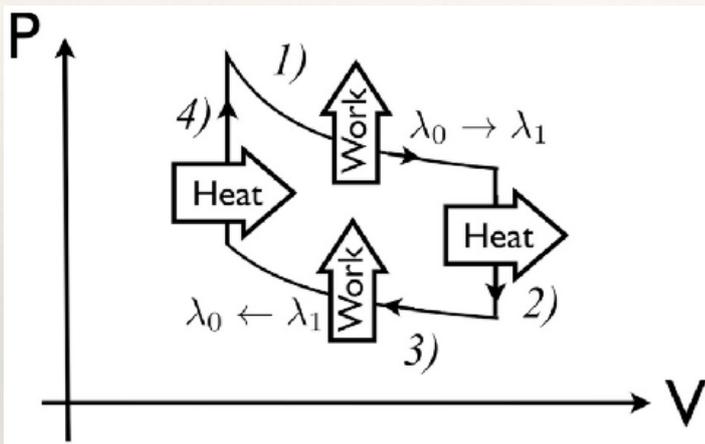
The Fundamental Physical Limits of Computation

What constraints govern the physical process of computing? Is a minimum amount of energy required, for example, per logic step? There seems to be no minimum, but some other questions are open

by Charles H. Bennett and Rolf Landauer

A computation, whether it is performed by electronic machinery, on an abacus or in a biological system such as the brain, is a physical process. It is subject to the same questions that apply to other physical processes: How much energy must be expended to perform a particular computation? How long must it take? How large must the computing device be? In other words, what are the physical limits of the process of computation?

So far it has been easier to ask these questions than to answer them. To the extent that we have found limits, they are terribly far away from the real limits of modern technology. We cannot profess, therefore, to be guiding the technologist or the engineer. What we are doing is really more fundamental. We are looking for general laws that must govern all information processing, no matter how it is accomplished. Any limits we find must be based solely on fundamental physical principles, not on whatever technology we may currently be using.

There are precedents for this kind of fundamental examination. In the 1940's Claude E. Shannon of the Bell Telephone Laboratories found there are limits on the amount of information that can be transmitted through a noisy channel; these limits apply no matter how the message is encoded into a signal. Shannon's work represents the birth of modern information science. Earlier, in the mid- and late 19th century, physicists attempting to determine the fundamental limits on the efficiency of steam engines had created the science of thermodynamics. In about 1960 one of us (Landauer) and John Swanson at IBM began attempting to apply the same type of analysis to the process of computing. Since the mid-1970's a growing number of other workers at other institutions have entered this field.

In our analysis of the physical limits of computation we use the term "information" in the technical sense of information theory. In this sense information is destroyed whenever two previously distinct situations become indistinguishable. In physical systems without friction, information can never be destroyed; whenever information is destroyed, some amount of energy must be dissipated (converted into heat). As an example, imagine two easily distinguishable physical situations, such as a rubber ball held either one meter or two meters off the ground. If the ball is dropped, it will bounce. If there is no friction and the ball is perfectly elastic, an observer will always be able to tell what state the ball started out in (that is, what its initial height was) because a ball dropped from two meters will bounce higher than a ball dropped from one meter.

If there is friction, however, the ball will dissipate a small amount of energy with each bounce, until it eventually stops bouncing and comes to rest on the ground. It will then be impossible to determine what the ball's initial state was; a ball dropped from two meters will be identical with a ball dropped from one meter. Information will have been lost as a result of energy dissipation.

Here is another example of information destruction: the expression $2 + 2$ contains more information than the expression $=4$. If all we know is that we have added two numbers to yield 4, then we do not know whether we have added $1 + 3$, $2 + 2$, $0 + 4$ or some other pair of numbers. Since the output is implicit in the input, no computation ever generates information.

In fact, computation as it is currently carried out depends on many operations that destroy information. The so-called *and* gate is a device with two input lines, each of which may be set at 1 or 0, and one output, whose value depends on the value of the inputs. If both inputs are 1, the output will be 1. If one of the inputs is 0 or if both are 0, the output will also be 0. Any time the gate's output is a 0 we lose information, because we do not know which of three possible states the input lines were in (0 and 1, 1 and 0, or 0 and 0). In fact, any logic gate that has more input than output lines inevitably discards information, because we cannot deduce the input from the output. Whenever we use such a "logically irreversible" gate, we dissipate energy into the environment. Erasing a bit of memory, another operation that is frequently used in computing, is also fundamentally dissipative; when we erase a bit, we lose all information about that bit's previous state.

Are irreversible logic gates and erasures essential to computation? If they are, any computation we perform has to dissipate some minimum amount of energy.

As one of us (Bennett) showed in 1973, however, they are not essential. This conclusion has since been demonstrated in several models; the easiest of these to describe are based on so-called reversible logic elements such as the Fredkin gate, named for Edward Fredkin of the Massachusetts Institute of Technology. The Fredkin gate has three input lines and three outputs. The input on one line, which is called the control channel, is fed unchanged through the gate. If the control channel is set at 0, the input on the other two lines also passes through unchanged. If the control line is a 1, however, the
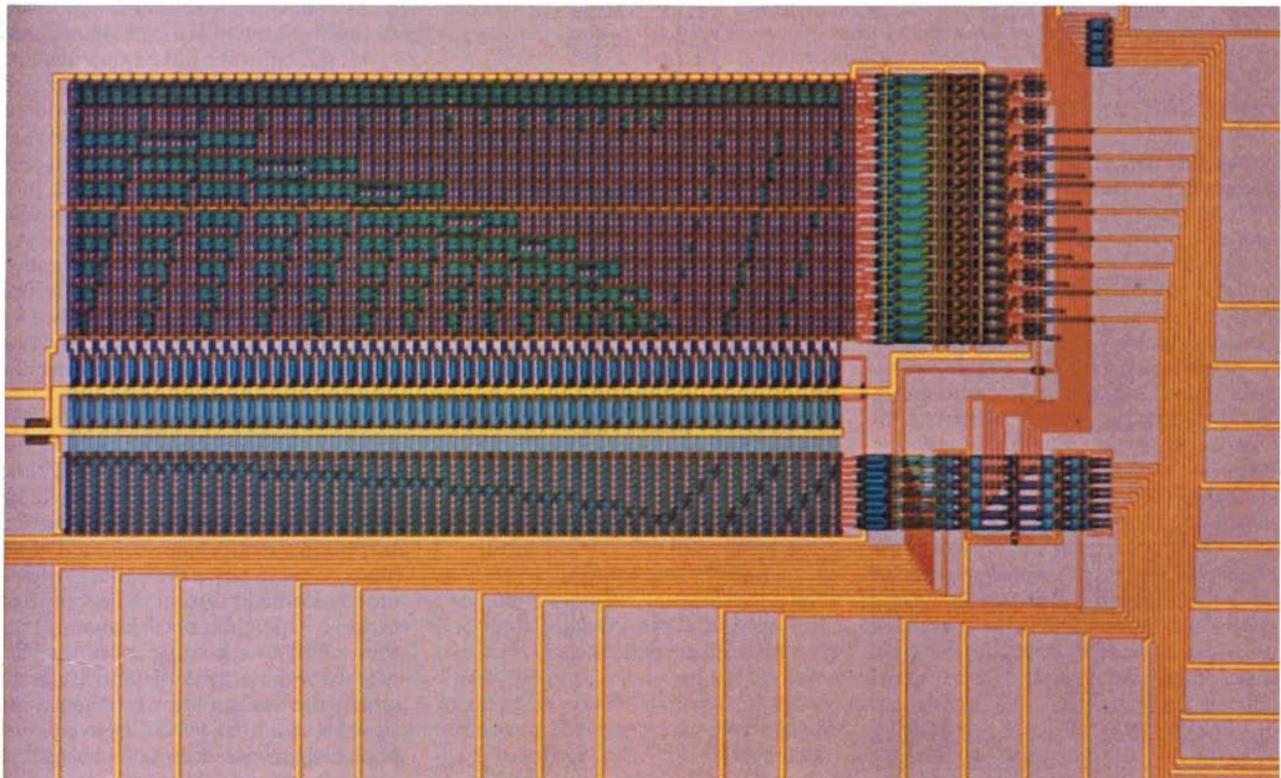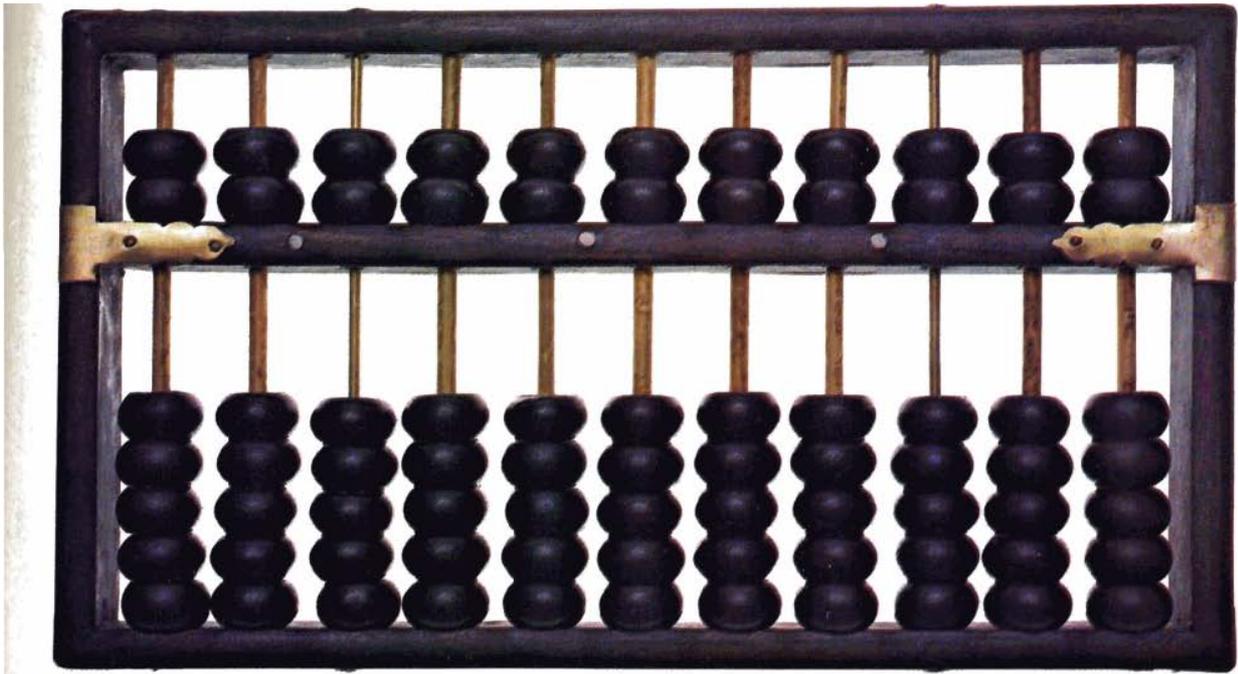
CONVENTIONAL COMPUTING DEVICES, the abacus and the logic chip, both dissipate energy when they are operated. The "logic gates" central to the design of a chip expend energy because they discard information. A chip consumes energy for a less fundamental reason as well: it employs circuits that draw power even when they merely hold information and do not process it. The abacus is dissipative because of friction between its beads and rods. It could not be built of frictionless components: if there were no static friction, the beads' positions would change under the influence of random thermal motion. Static friction exerts a certain minimum force no matter what the beads' velocity, and so there is some minium energy that the abacus requires no matter how slowly it is operated.

49

outputs of the other two lines are switched: the input of one line becomes the output of the other and vice versa. The Fredkin gate does not discard any information; the input can always be deduced from the output.

Fredkin has shown that any logic device required in a computer can be implemented by an appropriate arrangement of Fredkin gates. To make the computation work, certain input lines of some of the Fredkin gates must be preset at particular values *[see lower illustration below]*.

Fredkin gates have more output lines than the gates they are made to simulate. In the process of computing, what seem to be "garbage bits," bits of information that have no apparent use, are therefore generated. These bits must somehow be cleared out of the computer if we are to use it again, but if we erase them, it will cost us all the energy dissipation we have been trying to avoid.

Actually these bits have a most important use. Once we have copied down the result of our computation, which will reside in the normal output bits, we simply run the computer in reverse. That is, we enter the "garbage bits" and output bits that were produced by the computer's normal operation as "input" into the "back end" of the computer. This is possible because each of the logic gates in the computer is itself reversible. Running the computer in reverse discards no information, and so it need not dissipate any energy. Eventually the computer will be left exactly as it was before the computation began. Hence it is possible to complete a "computing cycle"— to run a computer and then to return it to its original state––without dissipating any energy.
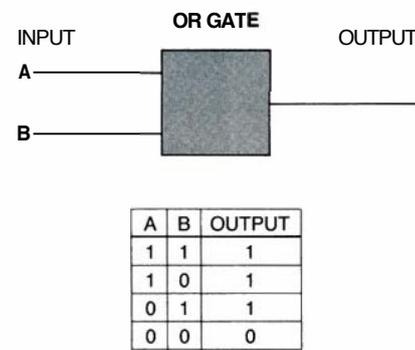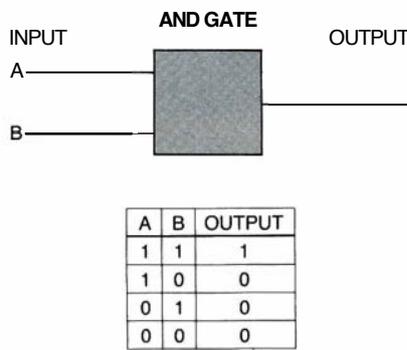
So far we have discussed a set of logic operations, not a physical device. It is not hard, however, to imagine a physical device that operates as a Fredkin gate. In this device the information channels are represented by pipes. A bit of information is represented by the presence or absence of a ball in a particular section of pipe; the presence of a ball signifies a 1 and the absence of a ball signifies a 0.
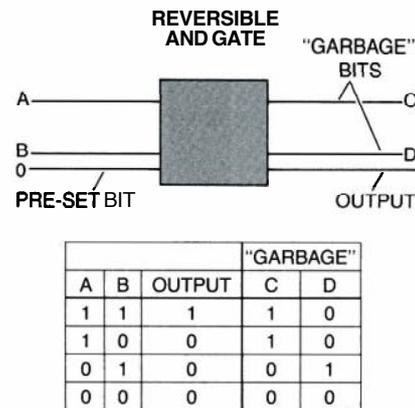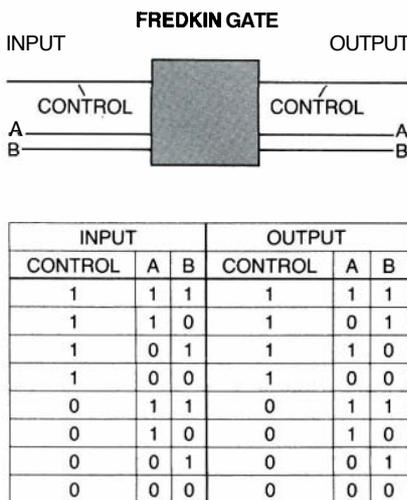
The control line is represented by a narrow segment of pipe that is split lengthwise down the middle. When a ball enters the split segment of pipe, it pushes the two halves of the pipe apart, actuating a switching device. The switching device channels any input balls that may be in the other two pipes: when a ball is present in the control line, any ball that enters an input pipe is automatically redirected to the other pipe. To ensure that the switch is closed when no control ball is present, there are springs that hold the two halves of the split pipe together. A ball entering the split pipe must expend energy when it compresses the springs, but this energy is not lost; it can be recovered when the control ball leaves the split pipe and the springs expand.

All the balls are linked together and pushed forward by one mechanism, so that they move in synchrony; otherwise we could not ensure that the various input and controlling balls would arrive at a logic gate together. In a sense the forward progress of the computation is really motion along a single degree of freedom, like the motion of two wheels rigidly attached to one axle. Once the computation is done we push all the balls backward, undoing all the operations and returning the computer to its initial state.

If the entire assembly is immersed in an ideal viscous fluid, then the frictional forces that act on the balls will be proportional to their velocity; there will be no static friction. The frictional force will therefore be very weak if we are content to move the balls slowly. In any mechanical system the energy that must be expended to work against friction is equal to the product of the frictional force and the distance through which the system travels. (Hence the faster a swimmer travels between two points, the more energy he or she will expend, although the distance traveled is the same whether the swimmer is fast or slow.) If we move the balls through the Fredkin gates at a low speed, then the energy expended (the product of force and distance) will be very small, because the frictional force depends directly on the balls' speed. In

AND GATE

INPUT — A, B → OUTPUT

A	B	OUTPUT
1	1	1
1	0	0
0	1	0
0	0	0

OR GATE

INPUT — A, B → OUTPUT

A	B	OUTPUT
1	1	1
1	0	1
0	1	1
0	0	0

CONVENTIONAL LOGIC GATES dissipate energy because they discard information. For example, if the output of an *and* gate is 0, there is no way to deduce what the input was.

FREDKIN GATE

INPUT — CONTROL, A, B → OUTPUT — CONTROL, A, B

INPUT			OUTPUT		
CONTROL	A	B	CONTROL	A	B
1	1	1	1	1	1
1	1	0	1	0	1
1	0	1	1	1	0
1	0	0	1	0	0
0	1	1	0	1	1
0	1	0	0	1	0
0	0	1	0	0	1
0	0	0	0	0	0

REVERSIBLE AND GATE

A, B, 0 (PRE-SET BIT) → "GARBAGE" BITS C, D, OUTPUT

A	B	OUTPUT	"GARBAGE"	
			C	D
1	1	1	1	0
1	0	0	1	0
0	1	0	0	1
0	0	0	0	0

FREDKIN REVERSIBLE LOGIC GATE need not dissipate energy; the input can always be deduced from the output. The gate has a "control" line, the value of which is not changed by the gate. If the bit on the control line is a 0, the values of the other two lines are also untouched; if it is a 1, however, the input of line A becomes the output of line B and vice versa. Reversible gates can be arranged to implement any function performed by an irreversible gate. To implement the *and* operation (right) one input is preset to equal 0, and two output bits, called garbage bits, are temporarily ignored. When the computation is complete, these bits are used to operate the gate in reverse, returning the computer to its original state.
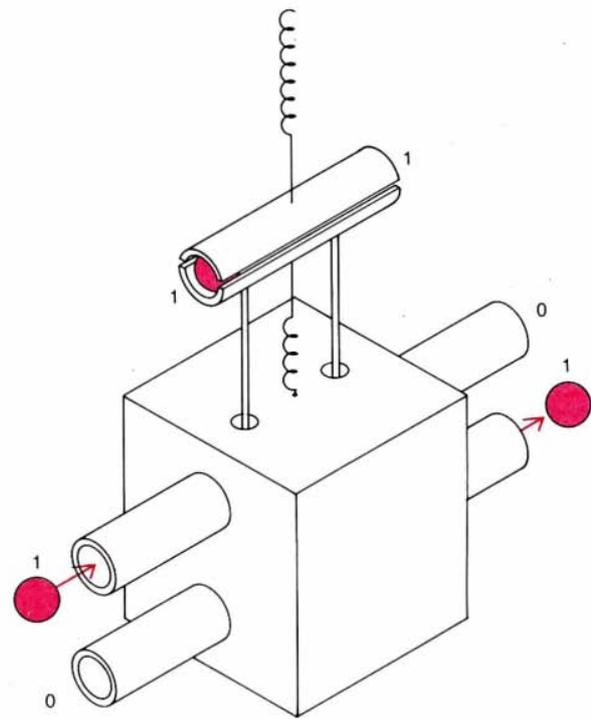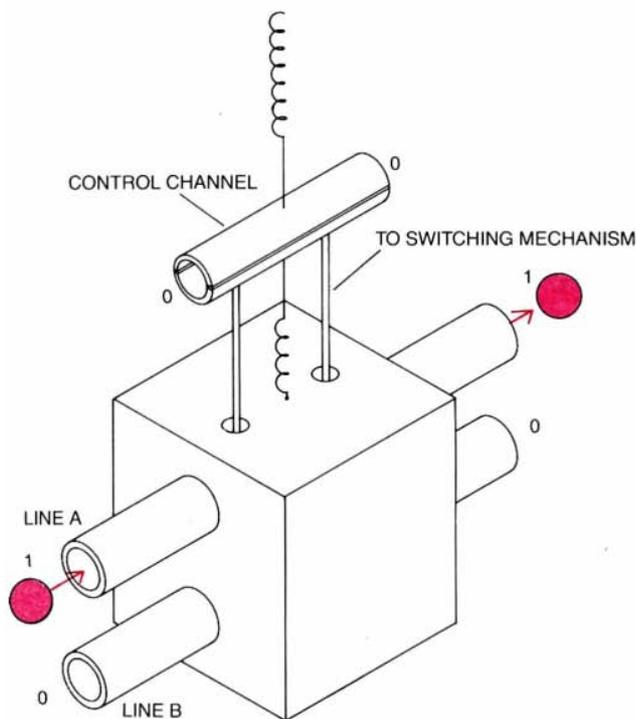
IDEALIZED PHYSICAL REALIZATION of a Fredkin gate substitutes pipes for wires and the presence or absence of a ball for a 1 or 0. A narrow, split segment of pipe represents the control channel. When a ball passes through it, the pipe spreads apart, operating a switching mechanism; the mechanism in turn switches any input ball from line A to line B and vice versa. A pair of springs keeps the control channel closed when no ball is in it. This gate does not need static friction in order to operate; it could be immersed in a viscous fluid, and the frictional forces could be made to depend only on the balls' velocity. Then the energy dissipation could be as small as the user wished: to lower the amount of energy dissipated, it would only be necessary to drive the balls through the device more slowly.

fact, we can expend as little energy as we wish, simply by taking a long time to carry out the operation. There is thus no minimum amount of energy that must be expended in order to perform any given computation.

The energy lost to friction in this model will be very small if the machine is operated very slowly. Is it possible to design a more idealized machine that could compute without any friction? Or is friction essential to the computing process? Fredkin, together with Tommaso Toffoli and others at M.I.T., has shown that it is not.

They demonstrated that it is possible to do computation by firing ideal, frictionless billiard balls at one another. In the billiard-ball model perfect reflecting "mirrors," surfaces that redirect the balls' motion, are arranged in such a way that the movement of the balls across a table emulates the movement of bits of information through logic gates *[see illustration on next page].* As before, the presence of a ball in a particular part of the computer signifies a 1, whereas the absence of a ball signifies a 0. If two balls arrive simultaneously at a logic gate, they will collide and their paths will change; their new paths represent the output of the gate. Fredkin, Toffoli and others have de-

scribed arrangements of mirrors that correspond to different types of logic gate, and they have shown that billiard-ball models can be built to simulate any logic element that is necessary for computing.

To start the computation we fire a billiard ball into the computer wherever we wish to input a 1. The balls must enter the machine simultaneously. Since they are perfectly elastic, they do not lose energy when they collide; they will emerge from the computer with the same amount of kinetic energy we gave them at the beginning.

In operation a billiard-ball computer produces "garbage bits," just as a computer built of Fredkin gates does. After the computer has reached an answer we reflect the billiard balls back into it, undoing the computation. They will come out of the machine exactly where we sent them in, and at the same speed. The mechanism that launched them into the computer can then be used to absorb their kinetic energy. Once again we will have performed a computation and returned the computer to its initial state without dissipating energy.

The billiard-ball computer has one major flaw: it is extremely sensitive to slight errors. If a ball is aimed slightly incorrectly or if a mirror is tilted at a

slightly wrong angle, the balls' trajectories will go astray. One or more balls will deviate from their intended paths, and in due course errors will combine to invalidate the entire computation. Even if perfectly elastic and frictionless billiard balls could be manufactured, the small amount of random thermal motion in the molecules they are made of would be enough to cause errors after a few dozen collisions.

Of course we could install some kind of corrective device that would return any errant billiard ball to its desired path, but then we would be obliterating information about the ball's earlier history. For example, we might be discarding information about the extent to which a mirror is tilted incorrectly. Discarding information, even to correct an error, can be done only in a system in which there is friction and loss of energy. Any correctional device must therefore dissipate some energy.

Many of the difficulties inherent in the billiard-ball computer can be made less extreme if microscopic or submicroscopic particles, such as electrons, are used in place of billiard balls. As Wojciech H. Zurek, who is now at the Los Alamos National Laboratory, has pointed out, quantum laws, which can restrict particles to a few states of motion, could eliminate the possibility

that a particle might go astray by a small amount.

Although the discussion so far has been based primarily on classical dynamics, several investigators have proposed other reversible computers that are based on quantum-mechanical principles. Such computers, first proposed by Paul Benioff of the Argonne National Laboratory and refined by others, notably Richard P. Feynman of the California Institute of Technology, have so far been described only in the most abstract terms. Essentially the particles in these computers would be arranged so that the quantum-mechanical rules governing their interaction would be precisely analogous to the rules describing the predicted outputs of various reversible logic gates. For example, suppose a particle's spin can have only two possible values: up

(corresponding to a binary 1) and down (corresponding to a 0). The interactions between particle spins can be prescribed in such a way that the value of one particle's spin changes depending on the spin of nearby particles; the spin of the particle would correspond to one of the outputs of a logic gate.

So far this discussion has concentrated on information processing. A computer must store information as well as process it. The interaction between storage and processing is best described in terms of a device called a Turing machine, for Alan M. Turing, who first proposed such a machine in 1936. A Turing machine can perform any computation that can be performed by a modern computer. One of us (Bennett) has shown that it is possible to build a reversible Turing ma-

chine: a Turing machine that does not discard information and can therefore be run with as small an expenditure of energy as the user wishes.

A Turing machine has several components. There is a tape, divided into discrete frames or segments, each of which is marked with a 0 or a 1; these bits represent the input. A "read/write head" moves along the tape. The head has several functions. It can read one bit of the tape at a time, it can print one bit onto the tape and it can shift its position by one segment to the left or right. In order to remember from one cycle to the next what it is doing, the head mechanism has a number of distinct "states"; each state constitutes a slightly different configuration of the head's internal parts.

In each cycle the head reads the bit on the segment it currently occupies;
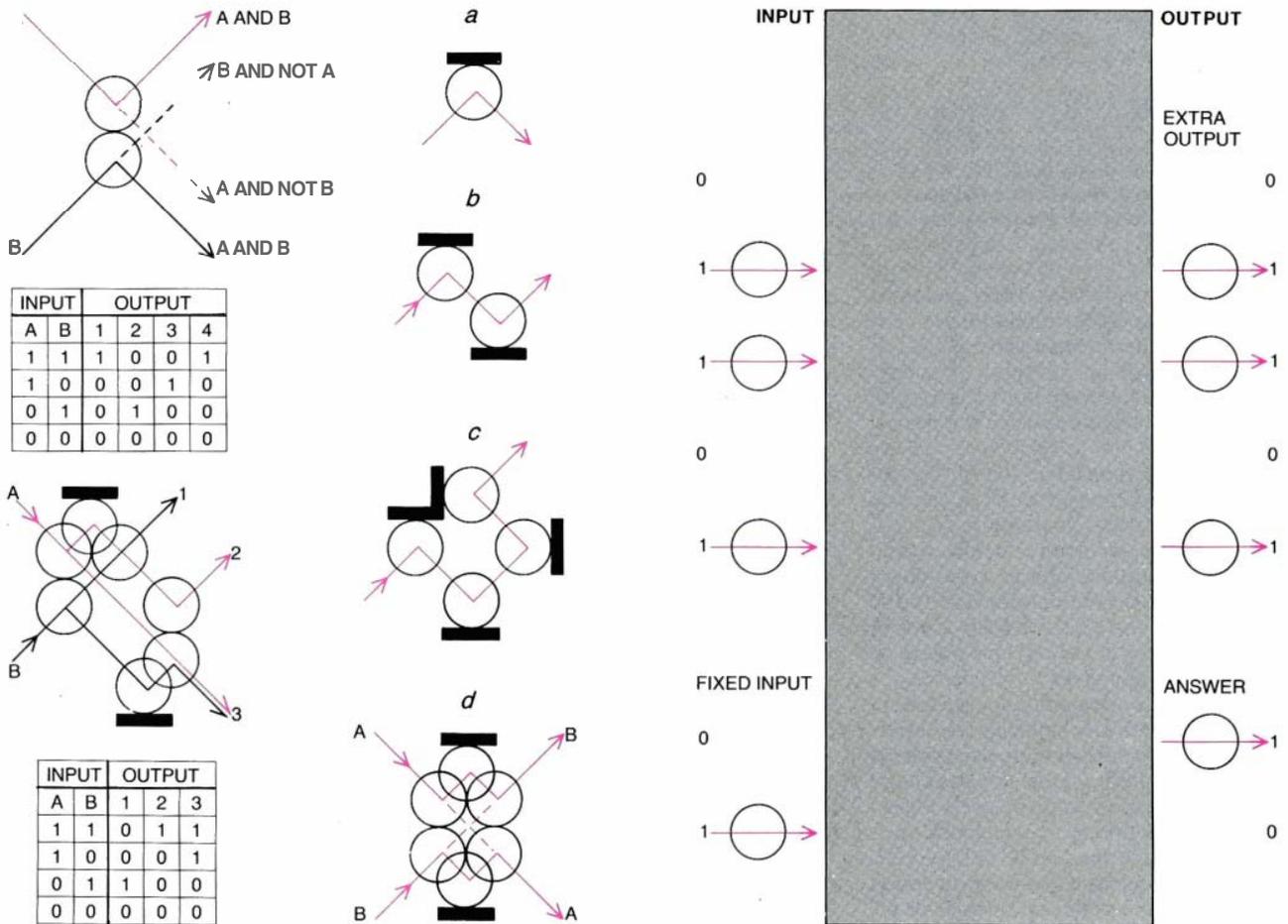
BILLIARD-BALL COMPUTER employs the movement of billiard balls on a table to simulate the movement of bits through logic gates. In billiard-ball logic gates (left) the balls' paths are redirected by collisions with one another or with reflecting "mirrors." In addition to their role in gates, mirrors can deflect a ball's path (a), shift the path sideways (b), delay the ball's motion without changing its final direction or position (c) or allow two lines to cross (d). It is possible to arrange mirrors so that the resulting "computer" implements the function of any logic chip. For example, a billiard-ball computer could be made to test whether a number is prime. One such computer (right) accepts as input any five-bit number (in this case 01101, or 13) and the fixed input sequence 01. Like a Fredkin gate, a billiard-ball computer typically returns more output bits than its user needs. In the case shown, the computer returns the original input number itself (which is the "extra" output), and an "answer" sequence: 10 if the input number is prime and 01 if it is composite.

then it prints a new bit onto the tape, changes its internal state and moves one segment to the left or right. The bit it prints, the state it changes into and the direction in which it moves are determined by a fixed set of transition rules. Each rule specifies a particular set of actions. Which rule the machine follows is determined by the state of the head and the value of the bit that it reads from the tape. For example, one rule might be: "If the head is in state *A* and is sitting on a segment of tape that is printed with a 0, it should change that bit to a 1, change its state to state B and move one segment to the right." It may happen that the transition rule instructs the machine not to change its internal state, not to print a new bit onto the tape or to halt its operation. Not all Turing machines are reversible, but a reversible Turing machine can be built to perform any possible computation.

The reversible Turing-machine models have an advantage over such machines as the frictionless billiard-ball computer. In the billiard-ball computer random thermal motion causes unavoidable errors. Reversible Turing-machine models actually exploit random thermal motion: they are constructed in such a way that thermal motion itself, with the assistance of a very weak driving force, moves the machine from one state to the next. The progress of the computation resembles the motion of an ion (a charged particle) suspended in a solution that is held in a weak electric field. The ion's motion, as seen over a short period of time, appears to be random; it is nearly as likely to move in one direction as in another. The applied force of the electric field, however, gives the net motion a preferred direction: the ion is a little likelier to move in one direction than in the other.

It may at first seem inconceivable that a purposeful sequence of operations, such as a computation, could be achieved in an apparatus whose direction of motion at any one time is nearly random. This style of operation is quite common, however, in the microscopic world of chemical reactions. There the trial-and-error action of Brownian motion, or random thermal motion, suffices to bring reactant molecules into contact, to orient and bend them into the specific conformation required for them to react, and to separate the product molecules after the reaction. All chemical reactions are in principle reversible: the same Brownian motion that accomplishes the forward reaction sometimes brings product molecules together and pushes them backward through the transition.
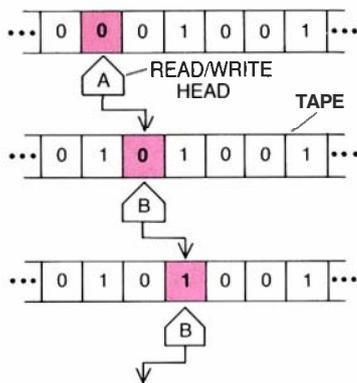
TURING MACHINE can be constructed in such a way that it can perform any computation a computer can. An infinitely long tape is divided into discrete segments, each of which bears either a 0 or a 1. A "read/write head," which can be in any of several internal states (here there are only two states, A and B), moves along the tape. Each cycle begins as the head reads one bit from a segment of the tape. Then, in accordance with a fixed set of transition rules, it writes a bit onto that segment, changes its own internal state and moves one segment to the left or right. This Turing machine, because it has only two head states, can do only trivial computations; more complicated machines with more head states are capable of simulating any computer, even one much more complicated than themselves. To do so they store a representation of the larger machine's complete logical state on the unlimited tape and break down each complex cycle into a large number of simple steps. The machine shown is logically reversible: it is always possible to deduce the machine's previous configuration. Other Turing machines, with different transition rules, are not reversible

In a state of equilibrium a backward reaction is just as likely to occur as a forward one.

In order to keep a reaction moving in the forward direction, we must supply reactant molecules and remove product molecules; in effect, we must provide a small driving force. When the driving force is very small, the reaction will take nearly as many backward steps as forward ones, but on the average it will move forward. In order to provide the driving force we must expend energy, but as in our ball-and-pipe realization of the Fredkin gate the total amount of energy can be as small as we wish; if we are willing to allow a long time for an operation, there is no minimum amount of energy that must be expended. The reason is that the total energy dissipated depends on the number of forward steps divided by the number of backward steps. (It is actually proportional to the logarithm of this ratio, but as the ratio increases or decreases so does its logarithm.) The slower the reaction moves forward, the smaller the ratio will be. (The analogy of the faster and slower swimmers is valid once again: it requires less total energy to go the same net number of reaction steps ,forward if the reaction moves slowly.)

We can see how a Brownian Turing machine might work by examining a Brownian tape-copying machine that already exists in nature: RNA polymerase, the enzyme that helps to construct RNA copies of the DNA constituting a gene. A single strand of DNA is much like the tape of a Turing machine. At each position along the strand there is one of four "bases": adenine, guanine, cytosine or thymine (abbreviated A, *G,* C and T). RNA is a similar chainlike molecule whose four bases, adenine, guanine, cytosine and uracil (A, *G,* C and U) bind to "complementary" DNA bases.

The RNA polymerase catalyzes this pairing reaction. The DNA helix is normally surrounded by a solution containing a large number of nucleoside triphosphate molecules, each consisting of an RNA base linked to a sugar and a tail of three phosphate groups. The RNA-polymerase enzyme selects from the solution a single RNA base that is complementary to the base about to be copied on the DNA strand. It then attaches the new base to the end of the growing RNA strand and releases two of the phosphates into the surrounding solution as a free pyrophosphate ion. Then the enzyme shifts forward one notch along the strand of DNA in preparation for attaching the next RNA base. The result is a strand of RNA that is complementary to the template strand of DNA. Without RNA polymerase this set of reactions would occur very slowly, and there would be little guarantee that the RNA and DNA molecules would be complementary.

The reactions are reversible: sometimes the enzyme takes up a free pyrophosphate ion, combines it with the last base on the RNA strand and re-

leases the resulting nucleoside triphosphate molecule into the surrounding solution, meanwhile backing up one notch along the DNA strand. At equilibrium, forward and backward steps would occur with equal frequency; normally other metabolic processes drive the reaction forward by removing pyrophosphate and supplying the four kinds of nucleoside triphosphate. In the laboratory the speed with which RNA polymerase acts can be varied by adjusting the concentrations of the reactants (as Judith Levin and Michael J. Chamberlin of the University of California at Berkeley have shown). As the concentrations are brought closer to equilibrium the enzyme works more slowly and dissipates less energy to copy a given section of DNA, because the ratio of forward to backward steps is smaller.

Although RNA polymerase merely copies information without processing it, it is relatively easy to imagine how a hypothetical chemical Turing machine might work. The tape is a single long backbone molecule to which two types of base, representing the binary 0 and 1, attach at periodic sites. A small additional molecule is attached to the 0 or 1 group at one site along the chain. The position of this additional molecule represents the position of the Turing machine's head. There are several different types of "head molecule," each type representing a different machine state.

The machine's transition rules are represented by enzymes. Each enzyme is capable of catalyzing one particular reaction. The way these enzymes work is best demonstrated by an example.

Suppose the head molecule is type A (indicating that the machine is in state A) and is attached to a 0 base. Also suppose the following transition rule applies: "When the head is in state A and reads a 0, change the 0 to a 1, change state to B and move to the right." A molecule of the enzyme representing this rule has a site that fits a type-A head molecule attached to a 1 base. It also has one site that fits a 0 base and one site that fits a B head [see illustration on opposite page].

To achieve the transition, the enzyme molecule first approaches the tape molecule at a location just to the right of the base on which the A head resides. Then it detaches from the tape both the head molecule and the 0 base to which the head was attached, putting in their place a 1 base. Next it attaches a B head to the base that is to the right of the 1 base it has just added to the tape. At this point the transition is complete. The head's original site is changed from a 0 to a 1, the head mole-

cule is now a type B, and it is attached to the base that is one notch to the right of the previous head position.

During the operation of a Brownian Turing machine the tape would have to be immersed in a solution containing many enzyme molecules, as well as extra 0's, 1's, A's and B's. To drive the reaction forward there would have to be some other reaction that cleaned the enzyme molecules of detached heads and bases. The concentrations of the reactants that clean the enzyme molecules represent the force that drives the Turing machine forward. Again we can expend as little energy as we wish simply by driving the machine forward very slowly.

The enzymatic Turing machine would not be error-free. Occasionally a reaction that is not catalyzed by any enzyme might occur; for example, a 0 base could spontaneously detach itself from the backbone molecule and a 1 base could be attached in its place. Similar errors do indeed occur during RNA synthesis.

In principle it would be possible to eliminate errors by building a Brownian Turing machine out of rigid, frictionless clockwork. The clockwork Turing machine involves less idealization than the billiard-ball computer but more than the enzymatic Turing machine. On the one hand, its parts need not be manufactured to perfect tolerances, as the billiard balls would have to be; the parts fit loosely together, and the machine can operate even in the presence of a large amount of thermal noise. Still, its parts must be perfectly rigid and free of static friction, properties not found in any macroscopic body.

Because the machine's parts fit together loosely, they are held in place not by friction but by grooves or notches in neighboring parts [see illustration on page 56]. Although each part of the machine is free to jiggle a little, like the pieces of a well-worn wood puzzle, the machine as a whole can only follow one "computational path." That is, the machine's parts interlock in such a way that at any time the machine can make only two kinds of large-scale motion: the motion corresponding to a forward computational step and that corresponding to a backward step.

The computer makes such transitions only as the accidental result of the random thermal motion of its parts biased by the weak external force. It is nearly as likely to proceed backward along the computational path, undoing the most recent transition, as it is to proceed forward. A small force, provided externally, drives the computation forward. This force can again be
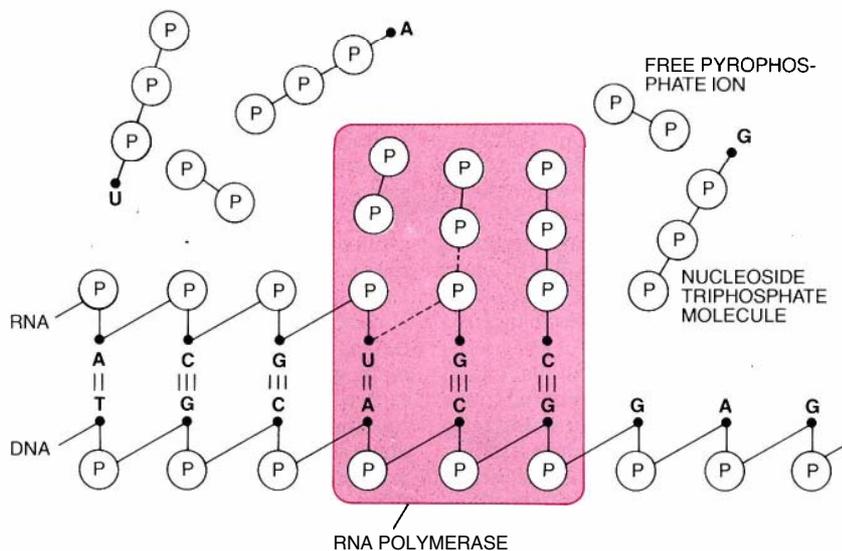
RNA POLYMERASE, an enzyme, acts as a reversible tape-copying machine; it catalyzes the reaction that constructs RNA copies of segments of DNA. As the enzyme moves along a strand of DNA, it selects from the surrounding solution a nucleoside triphosphate molecule (an RNA base bound to a sugar and a "tail" of three phosphate groups) that is complementary to the DNA base about to be copied. It then attaches the new base to the end of the RNA strand and releases a free pyrophosphate ion consisting of two phosphates. The reaction is reversible: sometimes the enzyme takes up the last link of RNA, attaches it to a pyrophosphate ion and returns the resulting molecule to the solution, backing up a notch on the DNA strand. When the reaction is close to chemical equilibrium, the enzyme takes almost as many backward as forward steps and the total energy needed to copy any segment of DNA is very small. The reaction can be made less dissipative by being run more slowly; there is no minimum amount of energy that must be expended to copy a segment of DNA.

as small as we wish, and so there is no minimum amount of energy that must be expended in order to run a Brownian clockwork Turing machine.

According to classical thermodynamics, then, there is no minimum amount of energy required in order to perform a computation. Is the classical thermodynamical analysis in conflict with quantum theory? After all, the quantum-mechanical uncertainty principle states there must be an inverse relation between our uncertainty about how long a process takes and our uncertainty about how much energy the process involves. Some investigators have suggested that any switching process occurring in a short period of time must involve a **minimum** expenditure of energy.

In fact the uncertainty principle does not require any minimum energy expenditure for a fast switching event. The uncertainty principle would be applicable only if we attempted to measure the precise time at which the event took place. Even in quantum mechanics extremely fast events can take place without any loss of energy. Our confidence that quantum mechanics allows computing without any minimum expenditure is bolstered when we remember that Benioff and others have developed models of reversible quantum-mechanical computers, which dissipate no energy and obey the laws of quantum mechanics.

Thus the uncertainty principle does not seem to **place** a fundamental limit on the **process** of computation; neither does classical thermodynamics. Does this mean there are no **physical** limitations to computing? Far from it. The real limitations are associated with questions that are much harder to answer than those we have asked in this article. For example, do elementary logic operations require some minimum amount of time? What is the smallest possible gadgetry that could accomplish such operations? Because scales of size and time are connected by the velocity of light, it is likely that these two questions have related answers. We may not be able to find these answers, however, until it is determined whether or not there is ,some ultimate graininess in the universal scales of time and length.

At the other extreme, how large can we make a computer memory? How many particles in the universe can we bring and keep together for that purpose? The maximum possible size of a computer memory limits the precision with which we can calculate. It will limit, for example, the number of decimal places to which we can calculate pi. The inevitable deterioration proc-
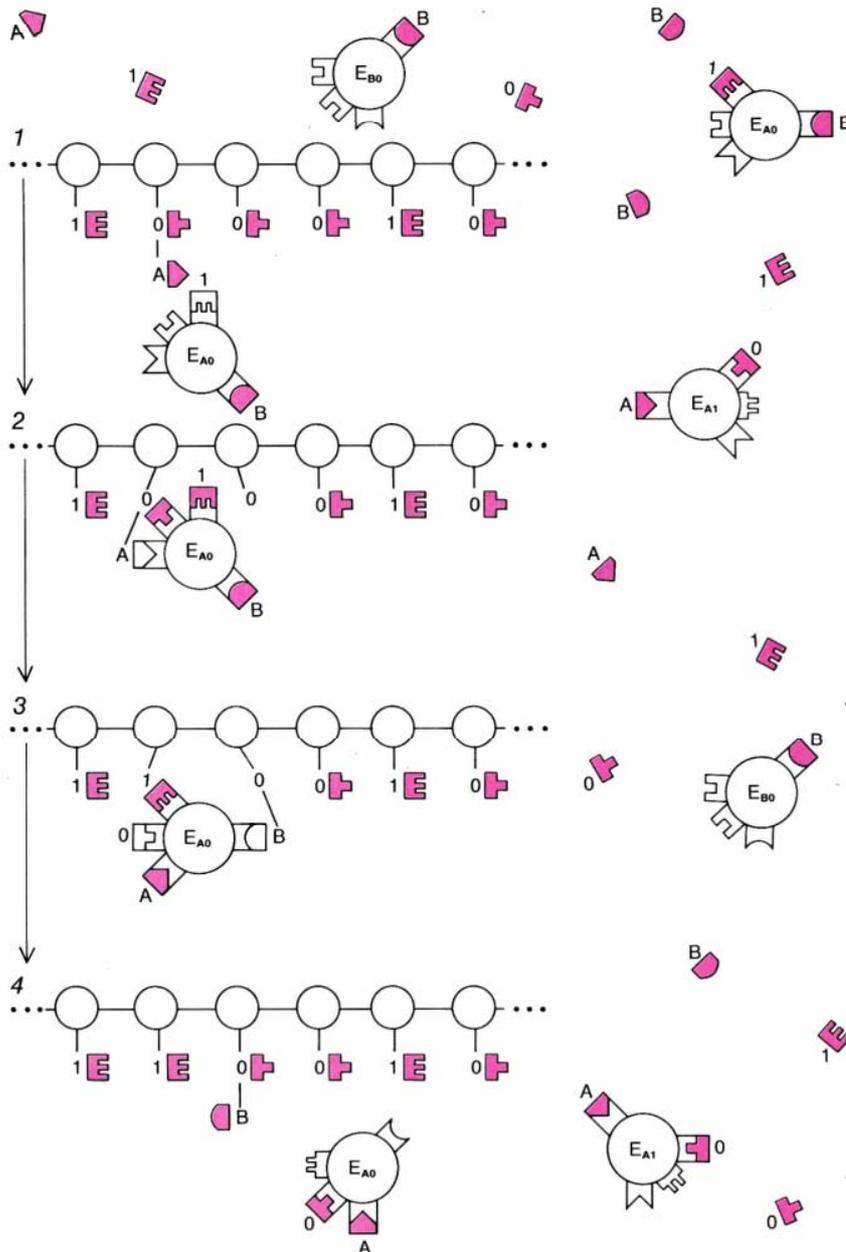
TRANSITION RULES				
HEAD STATE	BIT READ	CHANGE BIT TO	CHANGE STATE TO	MOVE TO
A	1	0	A	LEFT
A	0	1	B	RIGHT
B	1	1	A	LEFT
B	0	0	B	RIGHT

HYPOTHETICAL ENZYMATIC TURING MACHINE could perform a computation with no minimum expenditure of energy. Molecules representing 0 and 1 bits are attached at periodic intervals to a backbone molecule. A small additional molecule, representing the Turing machine's head, is attached to the 0 or 1 group at one site on the chain (I). There are several types of head molecule, each type representing a different internal machine state. Transition rules are represented by enzymes. In each cycle an enzyme attaches itself to the head molecule and the bit molecule to which the head **is** attached (2); then it detaches them from the chain, putting in their place the appropriate bit molecule (3). As it does so it rotates, so that it attaches the appropriate head molecule to the bit that occupies the site one notch to the right or left of the bit it has **just** changed. Now the cycle is complete (4): the value of a bit has been changed, and the head has changed state and shifted its position. **Each** kind of enzyme is **able** to catalyze one such set of reactions. As in the case of RNA synthesis, these reactions can be made to dissipate an **arbitrarily** small amount of energy.

esses that occur in real computers pose another, perhaps related, question: Can deterioration, at least in principle, be reduced to any desired degree, or does it impose a limit on the maximum length of time we shall be able to devote to any one calculation? That is, are there certain calculations that cannot be completed before the computer's hardware decays into uselessness?

Such questions really concern limi-*tations* on the physical execution of mathematical operations. Physical laws, on which the answers must ulti-mately be based, are themselves expressed in terms of such mathematical operations. Thus we are asking about the ultimate form in which the laws of physics can be applied, given the constraints imposed by the universe that the laws themselves describe.

TRANSITION RULES				
HEAD STATE	BIT READ	CHANGE BIT TO	CHANGE STATE TO	MOVE TO
A	1	0	A	LEFT
A	0	1	B	RIGHT
B	1	1	A	LEFT
B	0	0	B	RIGHT
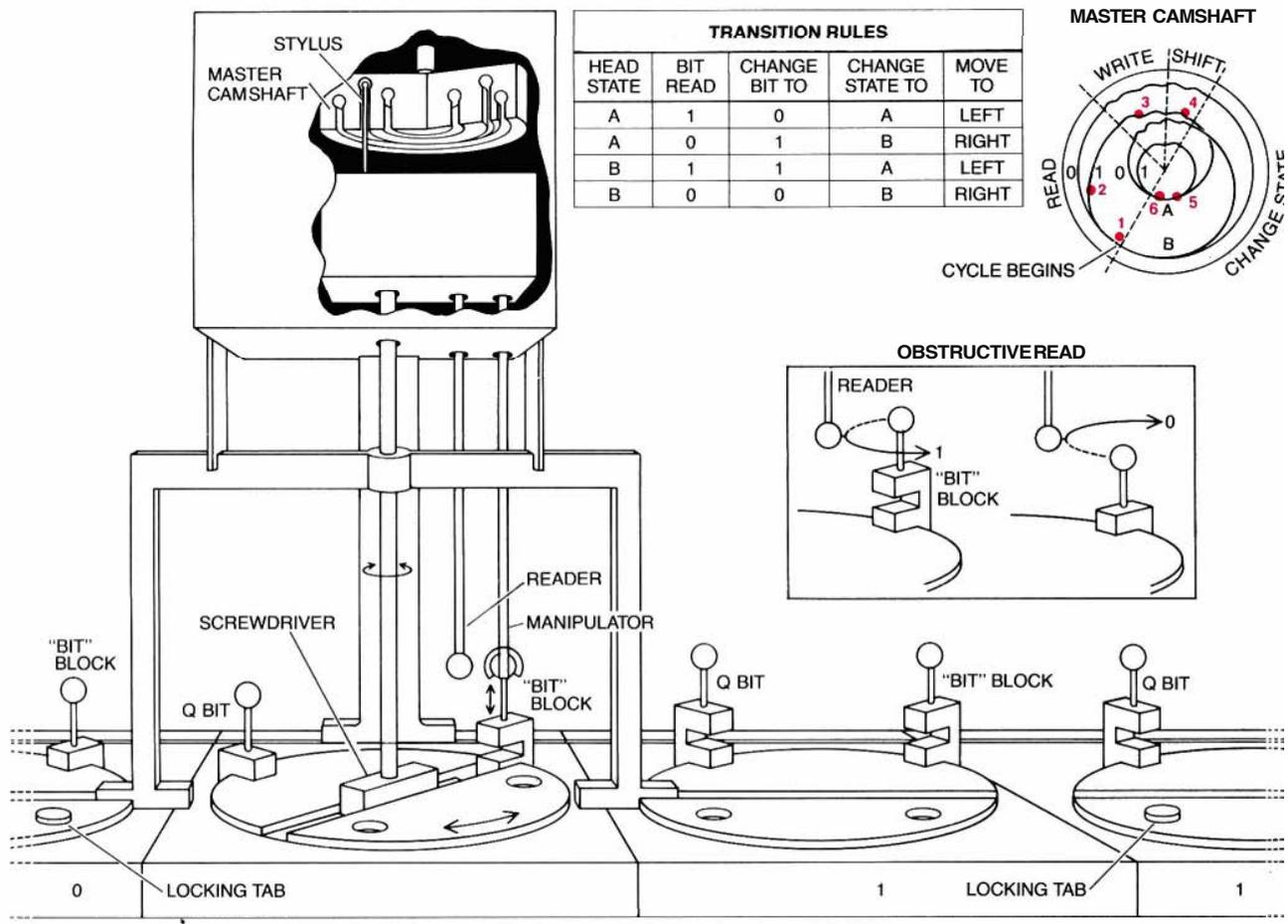
BROWNIAN CLOCKWORK TURING MACHINE, made out of rigid, frictionless parts, relies on random jiggling of its loosely fitted parts to change from state to state. When a part is held in place, it is not by friction **but** by grooves or notches in neighboring parts. Parts interlock in such a way that they can follow only one "computational patb"; although **they** are free to jiggle a little, the only large-scale motions they can make correspond to forward or backward computational steps. The operation of **the** machine is driven slowly forward by a very weak force; at any instant the machine is almost as likely to move backward as forward. On the average, however, the machine will move forward and the computation will eventually end. The machine can be made to dissipate as small an amount of energy as the user wishes, simply by employing a force of the correct weakness. Segments of tape are represented by grooved disks; bits are represented by E-shaped blocks, which are locked onto the disks in either the up (1)or the down (0) position. The head consists of a rigid framework and a complicated mechanism (most of which is not shown) from which are suspended a reader, a manipulator and a screwdriver-shaped rod. The machine's operation is controlled by a grooved "master camshaft," which resembles a phonograph record (top left and far right); different grooves correspond to different head states. At the beginning of a cycle the head is positioned above one of the disks and a **"stylus"** is in the "read" segment of the groove in the master camshaft that corresponds to the machine's current head state. During the **"read"** part of the cycle (*1*) the reader determines whether the disk's "bit* block is up or down by a process called an obstructive read (center right). In an obstructive read the reader moves past the block, following a high or a low path; one of the paths **will** be obstructed by the knob on the end of the block, and so there will be only one **path** for the reader to follow. At the point on the master camshaft that corresponds to this "decision" the grooves branch; each groove splits into two, and the stylus is guided into the groove that corresponds to the bit's value (2). Then the master camshaft **turns** until the stylus is in the "write" segment (3).In this segment each groove contains a different set of "instructions" for the machine to follow; the instructions are transmitted by a complex linkage between the stylus and the rest of the mechanim. If the instructions **call** for the bit's value to change, the manipulator moves over and grasps the knob; **then** the screwdriver rotates the disk until the block is free to move, the manipulator moves the block up or down and the screwdriver rotates the disk again to hold **the** block in place. After the stylus passes through the **"write"** segment of the master camshaft it enters the "shift" segment (4). Each groove in this segment contains instructions to move the head one segment to the left or right. Then the stylus enters the "change state" segment of the camshaft **(5), where** grooves merge in such a way that the stylus falls into the groove representing the next head state. The cycle is now complete (6). Disks adjacent to the one being read are held in place by the head's framework. Disks that are farther away are held by "locking tabs." The locking tab on each disk is coupled to a special bit, called the Q bit, on an adjacent disk. The linkages between Q bits and locking tabs are constructed so that **the** disk currently being read is free to move, while disks far to the right or left are held still.

Collective decoherence of cold atoms coupled to a Bose–Einstein condensate

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Collective decoherence of cold atoms coupled to a Bose–Einstein condensate

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Abstract. We examine the time evolution of cold atoms (impurities) interacting with an environment consisting of a degenerate bosonic quantum gas. The impurity atoms differ from the environment atoms, being of a different species. This allows one to superimpose two independent trapping potentials, each being effective only on one atomic kind, while transparent to the other. When the environment is homogeneous and the impurities are confined in a potential consisting of a set of double wells, the system can be described in terms of an effective spin-boson model, where the occupation of the left or right well of each site represents the two (pseudo)-spin states. The irreversible dynamics of such system is here studied exactly, i.e. not in terms of a Markovian master equation. The dynamics of one and two impurities is remarkably different in respect of the standard decoherence of the spin-boson system. In particular, we show: (i) the appearance of coherence oscillations, (ii) the presence of super and subdecoherent states that differ from the standard ones of the

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spin-boson model, and (iii) the persistence of coherence in the system at long times. We show that this behaviour is due to the fact that the pseudospins have an internal spatial structure. We argue that collective decoherence also prompts information about the correlation length of the environment. In a one-dimensional (1D) configuration, one can change even more strongly the qualitative behaviour of the dephasing just by tuning the interaction of the bath.

Contents

1. Introduction

The reasons for the great interest in the physics of ultracold atoms in recent years are manifold. On the one hand, experimentalists have reached an unprecedented control over the many-body atomic state with very stable optical potentials and by the use of Feshbach resonances, which allow one to change the scattering length of the atoms [1]. In this context, the tremendous experimental results that have been achieved include: the observation of the superfluid-Mott insulator transition for bosons [2], one-dimensional (1D) strongly interacting bosons in the Tonks–Girardeau regime [3] and Anderson localization [4, 5]. On the other hand, new experimental challenges come from different theoretical proposals for using this system for quantum information processing [6] and as a quantum simulator of condensed matter models (see for example [7]–[9] and references therein).

Not only can ultracold atoms simulate Hamiltonian systems, but such systems also offer a way to engineer non-classical environments. Thanks to the flexibility of quantum gases, a broad range of regimes of irreversible dynamics of open quantum systems and in particular of spin-boson systems can be explored [10]–[12].

In the present paper, we propose a new method by which an instance of the spin-boson model [13] can be realized with a suitable arrangement of interacting cold atoms. In particular, we analyse a system consisting of cold impurity atoms interacting with a degenerate quantum gas of a different atomic species. This setup makes possible the superposition of two independent trapping potentials, each being effective on one atomic species only, while transparent to the other. When the quantum gas is homogeneous and the impurities are confined

in a potential composed of double wells, the system can be described in terms of an effective spin-boson model, where occupations of the left or right well represent the two (pseudo)-spin states. At variance with other setups, where the role of the pseudospin is played by the presence or absence of one particle in a trapping well [14], by the vibrational modes of a single well [15] or by internal electronic levels [12], in our case each pseudospin has a spatial dimension, namely the separation between the two minima of the impurity double well. This introduces an effective suppression of the decoherence due to low-frequency modes of the environment and leads to unusual and interesting phenomena, like oscillations of coherence at finite times and the survival of coherence at long times. Further novel features appear when one considers the irreversible collective decoherence of a systems of two impurities. In this case, we still predict the existence of subdecoherent and superdecoherent states, but with the interesting fact that their role is exactly the opposite from what one observes in conventional spin-boson systems. Further interesting features appear when one considers how the collective decoherence rates change as a function of the impurities' separation and the effects of dimensionality of the system.

In discussing our investigations, for the sake of simplicity we shall consider an experimental setup where the impurity atoms are trapped by a periodic (optical) lattice. We would like to stress, however, that our findings do not depend on the lattice properties (e.g. periodicity) but on the numerical results. Other setups, such as microtraps on atom chips or quantum dots, just to mention a few, can be equally envisaged.

2. The Hamiltonian

Our system is composed of a cold quantum gas of bosonic atoms and a sample of cold atoms separated from each other and immersed in the quantum gas. In presenting our investigations, we shall use the words 'reservoir', 'bath' and 'environment' as synonyms to indicate the quantum gas, since its properties are not the focus of the present paper.

The second-quantized form of the Hamiltonian of the impurities + bath system takes the form (see also [16])

$$\hat{H} = \hat{H}_A + \hat{H}_B + \hat{H}_{AB}, \tag{1}$$

where

$$\hat{H}_A = \int d^3x \ \hat{\Psi}^\dagger(\mathbf{x}) \left[\frac{\mathbf{p}_A^2}{2m_A} + V_A(\mathbf{x}) \right] \hat{\Psi}(\mathbf{x}) \tag{2}$$

is the Hamiltonian of atomic impurities, described by the field operator $\hat{\Psi}(\mathbf{x})$ in the trapping potential $V_A(\mathbf{x})$, which creates a set of double wells of size $2L$ and separated by a distance $2D$, see figure 1,

$$\hat{H}_B = \int d^3x \ \hat{\Phi}^\dagger(\mathbf{x}) \left[\frac{\mathbf{p}^2}{2m_B} + V_B(\mathbf{x}) + \frac{g_B}{2} \ \hat{\Phi}^\dagger(\mathbf{x})\hat{\Phi}(\mathbf{x}) \right] \hat{\Phi}(\mathbf{x}) \tag{3}$$

is the Hamiltonian of the bath, composed of $N \gg 1$ bosons, represented by the field operator $\hat{\Phi}(\mathbf{x})$ and confined by a trapping potential $V_B(\mathbf{x})$ and $g_B = 4\pi\hbar^2 a_B/m_B$ is the boson–boson coupling constant, with a_B the scattering length of the condensate atoms, and

$$\hat{H}_{AB} = g_{AB} \int d^3x \ \hat{\Psi}^\dagger(\mathbf{x})\hat{\Phi}^\dagger(\mathbf{x})\hat{\Phi}(\mathbf{x})\hat{\Psi}(\mathbf{x}) \tag{4}$$

IOP Institute of Physics Φ DEUTSCHE PHYSIKALISCHE GESELLSCHAFT
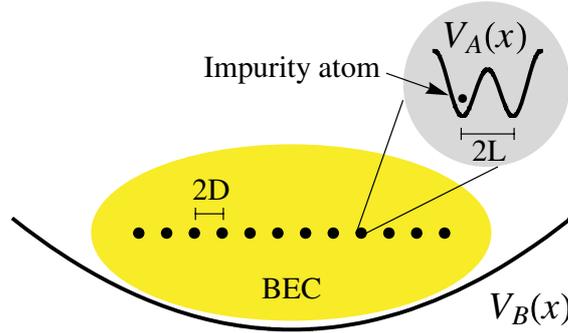
Figure 1. A Bose–Einstein condensate (yellow region) confined in a shallow harmonic trap $V_B(x)$ interacts with cold impurity atoms each of which is trapped in a double well potential $V_A(x)$ (grey circle). The distance between two wells in the same trap is 2L and the distance between adjacent traps is 2D.

describes the interactions between the impurities and the bath; here $g_{AB} = 2\pi\hbar^2 a_{AB}/m_{AB}$ is the coupling constant of impurities–gas interaction, with a_{AB} the scattering length of the impurities–gas collisions and $m_{AB} = m_A m_B/(m_A + m_B)$ their reduced mass. Both impurity and bath atoms are described in the second-quantized formalism. The field operator of the atomic impurities

$$\hat{\Psi}(\mathbf{x}) = \sum_{i,p} \hat{a}_{i,p} \varphi_{i,p}(\mathbf{x}) \tag{5}$$

can be decomposed in terms of the real eigenstates $\varphi_{i,p}(\mathbf{x})$ of impurity atoms localized on the double well i of the potential $V_A(x)$ in the pth state, with energy $\hbar\omega_{i,p}$ and the corresponding annihilation operator $\hat{a}_{i,p}$. We assume that the wavefunctions of different double wells have a negligible common support, i.e. $\varphi_{i,p}(\mathbf{x})\varphi_{j\neq i,m}(\mathbf{x}) \simeq 0$ at any position $\mathbf{x}$.

We treat the gas of bosons following Bogoliubov's approach (see, for instance, [17]) and assuming a very shallow trapping potential $V_B(\mathbf{x})$, such that the bosonic gas can be considered homogeneous. In the degenerate regime, the bosonic field can be decomposed as

$$\hat{\Phi}(\mathbf{x}) = \sqrt{N_0}\,\Phi_0(\mathbf{x}) + \delta\hat{\Phi}(\mathbf{x}) = \sqrt{N_0}\,\Phi_0(\mathbf{x}) + \sum_{\mathbf{k}} \left(u_{\mathbf{k}}(\mathbf{x})\hat{c}_{\mathbf{k}} - v_{\mathbf{k}}^*(\mathbf{x})\hat{c}_{\mathbf{k}}^\dagger \right), \tag{6}$$

where $\Phi_0(\mathbf{x})$ is the condensate wave function (or order parameter), $N_0 < N$ is the number of atoms in the condensate and $\hat{c}_{\mathbf{k}}$, $\hat{c}_{\mathbf{k}}^\dagger$ are the annihilation and creation operators of the Bogoliubov modes with momentum $\mathbf{k}$. For a homogeneous condensate $\Phi_0(\mathbf{x}) = 1/\sqrt{V}$, V being the volume. Its Bogoliubov modes

$$u_{\mathbf{k}} = \sqrt{\frac{1}{2}\left(\frac{\epsilon_{\mathbf{k}} + n_0 g_B}{E_{\mathbf{k}}} + 1\right)}\,\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}}, \tag{7}$$

$$v_{\mathbf{k}} = \sqrt{\frac{1}{2}\left(\frac{\epsilon_{\mathbf{k}} + n_0 g_B}{E_{\mathbf{k}}} - 1\right)}\,\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} \tag{8}$$

have energy

$$E_{\mathbf{k}} = \left[2\epsilon_{\mathbf{k}} n_0 g_{\mathrm{B}} + \epsilon_{\mathbf{k}}^2\right]^{1/2}, \tag{9}$$

where $\epsilon_{\mathbf{k}} = \hbar^2 k^2/(2m_{\mathrm{B}})$ and $n_0 = N_0/V$ is the condensate density. As one can see from (9), low-energy excitations have phonon-like (wave-like) spectrum, whereas high-energy excitations have particle-like spectrum. The condition for wave-like excitations is $\epsilon_{\mathbf{k}} \ll n_0 g_{\mathrm{B}}$, i.e. $k \ll 4\sqrt{\pi n_0 a_{\mathrm{B}}}$, or equivalently $k \ll 2m_{\mathrm{B}} c_{\mathrm{s}}/\hbar$, where $c_{\mathrm{s}} = \sqrt{n_0 g_{\mathrm{B}}/m}$ is the speed of sound at zero temperature. Note that $|u_{\mathbf{k}}| = 1/\sqrt{V}$ and $|v_{\mathbf{k}}| = 0$ describe the limiting case of $N \gg 1$ non-interacting bosons, each with energy $E_{\mathbf{k}} = \epsilon_{\mathbf{k}}$.

Inserting equations (5) and (6) into the Hamiltonian (1) we obtain

$$\hat{H}_{\mathrm{A}} = \sum_{i,p} \hbar\omega_{i,p} \hat{a}_{i,p}^{\dagger} \hat{a}_{i,p} \tag{10}$$

for the impurities,

$$\hat{H}_{\mathrm{B}} = H_{\mathrm{Cond}} + \hat{H}_{\mathrm{Bog}} \tag{11}$$

for the quantum gas, with

$$H_{\mathrm{Cond}} = N_0 \int \mathrm{d}^3 x \; \Phi_0^*(\mathbf{x}) \left[\frac{\mathbf{p}^2}{2m_{\mathrm{B}}} + V^B(\mathbf{x}) + \frac{g_{\mathrm{B}}}{2} N_0 |\Phi_0(\mathbf{x})|^2 \right] \Phi_0(\mathbf{x}) \tag{12}$$

for the condensate and

$$\hat{H}_{\mathrm{Bog}} = \sum_{\mathbf{k}} E_{\mathbf{k}} \hat{c}_{\mathbf{k}}^{\dagger} \hat{c}_{\mathbf{k}} \tag{13}$$

for the collective excitations (Bogoliubov modes) of energy $E_{\mathbf{k}}$ in the condensate, and

$$\hat{H}_{\mathrm{AB}} = g_{\mathrm{AB}} \sum_{i} \sum_{p,q} \hat{a}_{i,p}^{\dagger} \hat{a}_{i,q} \left[N_0 \int \mathrm{d}^3 x \varphi_{i,p}(\mathbf{x}) \varphi_{i,q}(\mathbf{x}) |\Phi_0(\mathbf{x})|^2 \right.$$

$$+ \sqrt{N_0} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}} \int \mathrm{d}^3 x \varphi_{i,p}(\mathbf{x}) \varphi_{i,q}(\mathbf{x}) \left(\Phi_0^*(\mathbf{x}) u_{\mathbf{k}}(\mathbf{x}) - \Phi_0(\mathbf{x}) v_{\mathbf{k}}(\mathbf{x}) \right)$$

$$\left. + \sqrt{N_0} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}}^{\dagger} \int \mathrm{d}^3 x \varphi_{i,p}(\mathbf{x}) \varphi_{i,q}(\mathbf{x}) \left(\Phi_0(\mathbf{x}) u_{\mathbf{k}}^*(\mathbf{x}) - \Phi_0^*(\mathbf{x}) v_{\mathbf{k}}^*(\mathbf{x}) \right) \right] \tag{14}$$

for the interaction Hamiltonian; the terms that are quadratic in the Bogoliubov excitation operators $\hat{c}, \hat{c}^{\dagger}$ give negligible contributions and have been omitted. The first term in (14) describes transitions between impurities' vibrational states due to the condensate, whereas the remaining terms describe similar transitions induced by the collective excitations in the condensate. In a homogeneous condensate, transitions between different vibrational eigenstates

of the impurities induced by the condensate are suppressed, while all vibrational states $\varphi_{i,p}(\mathbf{x})$ get an energy shift $\delta\omega_{i,p}$,

$$g^{AB} N_0 \int d^3x \, |\Phi_0|^2(\mathbf{x}) \varphi_{i,p}(\mathbf{x}) \varphi_{i,q}(\mathbf{x}) = \begin{cases} 0, & \text{for } p \neq q, \\ n_0 g^{AB} \equiv \delta\omega_{i,p}, & \text{for } p = q \end{cases} \tag{15}$$

so the contribution of the first term in (14) can be included in the definition of $\omega_{i,p}$.

In the limit of deep, symmetric wells in each double well and separated by a high-energy barrier, the tunnelling between the adjacent wells is suppressed. In this regime, the ground states $\varphi_{i,L}$ and $\varphi_{i,R}$ of, respectively, the left and right wells of double well i are well separated in space with vanishing spatial overlap, their coupling to the excited states becomes negligible and the total Hamiltonian further simplifies into

$$\hat{H} = \sum_{i,\,p=L,R} \hbar\omega_{i,p}\hat{n}_p^i + \sum_{\mathbf{k}} E_{\mathbf{k}}\hat{c}_{\mathbf{k}}^\dagger\hat{c}_{\mathbf{k}} + \sum_i \hbar \sum_{p=L,R} \sum_{\mathbf{k}} \left[\Omega_{p,\mathbf{k}}^i \hat{c}_{\mathbf{k}} + \Omega_{p,\mathbf{k}}^{i*}\hat{c}_{\mathbf{k}}^\dagger \right] \hat{n}_p^i, \tag{16}$$

where we have defined the coupling frequencies

$$\Omega_{p,\mathbf{k}}^i \equiv \frac{g_{AB}\sqrt{n_0}}{\hbar} \left(|u_{\mathbf{k}}| - |v_{\mathbf{k}}| \right) \int d^3x \, |\varphi_{i,p}(\mathbf{x})|^2 e^{i\mathbf{k}\cdot\mathbf{x}} \tag{17}$$

and $\hat{n}_p^i \equiv \hat{a}_{i,p}^\dagger \hat{a}_{i,p}$ is the number operator of impurities in the double well i in the well $p = L, R$.

We consider the case where each double well is occupied by at most one impurity atom. This allows us to describe the occupation of the left and right wells of each site in terms of pseudospin states. Introducing the Pauli operators as $\hat{n}_L^i = (1 - \hat{\sigma}_z^i)/2$, $\hat{n}_R^i = (1 + \hat{\sigma}_z^i)/2$, the Hamiltonian (16) takes the form of the independent boson model [18]

$$\hat{H} = \sum_{\mathbf{k}} E_{\mathbf{k}}\hat{c}_{\mathbf{k}}^\dagger\hat{c}_{\mathbf{k}} + \frac{\hbar}{2} \sum_{\mathbf{k}} \left\{ \left[\sum_i \left(\Omega_{R,\mathbf{k}}^i - \Omega_{L,\mathbf{k}}^i \right) \hat{\sigma}_z^i + \sum_i \left(\Omega_{R,\mathbf{k}}^i + \Omega_{L,\mathbf{k}}^i \right) \right] \hat{c}_{\mathbf{k}} \right.$$

$$\left. + \left[\sum_i \left(\Omega_{R,\mathbf{k}}^{i*} - \Omega_{L,\mathbf{k}}^{i*} \right) \hat{\sigma}_z^i + \sum_i \left(\Omega_{R,\mathbf{k}}^{i*} + \Omega_{L,\mathbf{k}}^{i*} \right) \right] \hat{c}_{\mathbf{k}}^\dagger \right\}, \tag{18}$$

where a constant energy shift has been omitted. We note that spin-boson systems with larger spin values can be realized in the same way with higher occupation of the double wells.

The effects due to quantum noise on coherent superpositions of states of a double well spin-boson Hamiltonian have been analysed in the Markovian regime. In [19]–[21] the effects of a cold atom reservoir has been analysed, while [22] has considered the effects of scattered photons, taking into account also the role of the inter-well separation. As we will show in the following section, for our system it is possible to carry out a full analysis of the impurity dynamics, going beyond the Markov approximation.

3. Exact reduced impurities dynamics

The dynamics due to the spin-boson Hamiltonian (18) is amenable to an exact analytical solution and is characterized by decoherence without dissipation [23]–[25]. The time-evolution operator

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$\hat{U}(t) = \exp[-i\hat{H}t/\hbar]$ corresponding to the Hamiltonian (18) can be factorized into a product of simpler exponential operators,

$$\hat{U}(t) = \exp\left[-\frac{i}{\hbar}\sum_{\mathbf{k}} E_{\mathbf{k}}\hat{c}_{\mathbf{k}}^{\dagger}\hat{c}_{\mathbf{k}}t\right]$$

$$\times \exp\left[\sum_{\mathbf{k}}\left(\sum_{i} A_{\mathbf{k}}^{i}(t)\hat{\sigma}_{z}^{i} + \alpha_{\mathbf{k}}(t)\right)\hat{c}_{\mathbf{k}}^{\dagger} - \sum_{\mathbf{k}}\left(\sum_{i} A_{\mathbf{k}}^{i*}(t)\hat{\sigma}_{z}^{i} + \alpha_{\mathbf{k}}^{*}(t)\right)\hat{c}_{\mathbf{k}}\right]$$

$$\times \exp\left[i\hbar^2\sum_{\mathbf{k}} f_{\mathbf{k}}(t)\Re\sum_{ij}\frac{\left(\Omega_{R,\mathbf{k}}^{i} - \Omega_{L,\mathbf{k}}^{i}\right)\left(\Omega_{R,\mathbf{k}}^{j*} - \Omega_{L,\mathbf{k}}^{j*}\right)}{4E_{\mathbf{k}}^2}\hat{\sigma}_{z}^{i}\hat{\sigma}_{z}^{j}\right]$$

$$\times \exp\left[i\hbar^2\sum_{\mathbf{k}} f_{\mathbf{k}}(t)\Re\sum_{i}\frac{\left(\Omega_{R,\mathbf{k}}^{i} - \Omega_{L,\mathbf{k}}^{i}\right)\sum_{j}\left(\Omega_{R,\mathbf{k}}^{j*} + \Omega_{L,\mathbf{k}}^{j*}\right)}{2E_{\mathbf{k}}^2}\hat{\sigma}_{z}^{i}\right]$$

$$\times \exp\left[i\hbar^2\sum_{\mathbf{k}} f_{\mathbf{k}}(t)\frac{\sum_{i}\left(\Omega_{R,\mathbf{k}}^{i} + \Omega_{L,\mathbf{k}}^{i}\right)\sum_{j}\left(\Omega_{R,\mathbf{k}}^{j*} + \Omega_{L,\mathbf{k}}^{j*}\right)}{4E_{\mathbf{k}}^2}\right], \quad (19)$$

where the functions

$$f_{\mathbf{k}}(t) = \frac{E_{\mathbf{k}}}{\hbar}t - \sin\frac{E_{\mathbf{k}}}{\hbar}t, \quad (20)$$

$$A_{\mathbf{k}}^{i}(t) = \frac{\hbar\left(1 - e^{iE_{\mathbf{k}}t/\hbar}\right)}{2E_{\mathbf{k}}}\left(\Omega_{R,\mathbf{k}}^{i*} - \Omega_{L,\mathbf{k}}^{i*}\right), \quad (21)$$

$$\alpha_{\mathbf{k}}(t) = \frac{\hbar\left(1 - e^{iE_{\mathbf{k}}t/\hbar}\right)}{2E_{\mathbf{k}}}\sum_{i}\left(\Omega_{R,\mathbf{k}}^{i*} + \Omega_{L,\mathbf{k}}^{i*}\right), \quad (22)$$

have been introduced for ease of notation. Details of the derivation of (19) for the time-evolution operator are given in appendix A. As in this paper, we are interested in the irreversible collective decoherence of the impurities we will focus our attention on the conditional displacement operator

$$\hat{U}_{D}(t) = \prod_{\mathbf{k}}\hat{U}_{\mathbf{k},D}(t), \quad (23)$$

$$\hat{U}_{\mathbf{k},D}(t) \equiv \exp\left[\left(\sum_{i} A_{\mathbf{k}}^{i}(t)\hat{\sigma}_{z}^{i} + \alpha_{\mathbf{k}}(t)\right)\hat{c}_{\mathbf{k}}^{\dagger} - \left(\sum_{i} A_{\mathbf{k}}^{i*}(t)\hat{\sigma}_{z}^{i} + \alpha_{\mathbf{k}}^{*}(t)\right)\hat{c}_{\mathbf{k}}\right]. \quad (24)$$

Indeed this operator is the one responsible of the decoherence of impurities as it induces entanglement between them and the reservoir. Labelling the state of the impurities as $|\{n_p\}\rangle = |\{n_1, n_2, n_3, \ldots\}\rangle$ with $n_p = 0, 1$ denoting the presence of the atom, respectively, in the left or right well, the matrix elements of reduced density operator of the impurities are

$$\rho_{\{n_p\},\{m_p\}}(t) = \exp\left[-\Gamma_{\{n_i\},\{m_i\}}(t)\right]\rho_{\{n_p\},\{m_p\}}(0)\exp\left\{i\Theta_{\{n_p\},\{m_p\}}(t)\right\}$$

$$\times \exp\left\{i\Xi_{\{n_p\},\{m_p\}}(t)\right\}\exp\left\{i\Delta_{\{n_p\},\{m_p\}}(t)\right\}. \quad (25)$$

Assuming that each mode of the bosonic environment is in a mixed state $\rho_{\mathbf{k}}$ at equilibrium at temperature T the decay exponent contains all the information concerning the time dependence of the decoherence process and takes the form

$$\Gamma_{\{n_i\},\{m_i\}}(t) = \hbar^2 \sum_{\mathbf{k}} \frac{\left(1 - \cos \frac{E_{\mathbf{k}}}{\hbar} t\right)}{E_{\mathbf{k}}^2} \left| \sum_i [m_i - n_i] \left(\Omega_{\mathrm{R},\mathbf{k}}^i - \Omega_{\mathrm{L},\mathbf{k}}^i\right) \right|^2 \coth \frac{\beta E_{\mathbf{k}}}{2} \tag{26}$$

with $\beta = 1/K_{\mathrm{B}}T$. The phase factors $\Theta_{\{n_p\},\{m_p\}}(t)$, $\Xi_{\{n_p\},\{m_p\}}(t)$ and $\Delta_{\{n_p\},\{m_p\}}(t)$, whose specific form is given in appendix B, do not play any role in the decoherence [26]. They contain, however, interesting information on the effective coupling between the pseudospins induced by the condensate and will be analysed in a future paper [27].

4. Results for the decoherence

As mentioned in the introduction, we shall assume that the impurity atoms are trapped by an optical (super)lattice, whose form can be controlled and varied in time with great accuracy [28, 29]. The coupling frequencies $\Omega_{p,\mathbf{k}}^i$ are accordingly evaluated in appendix C assuming an optical lattice, with identical, double wells in each site, and deep trapping of impurity atoms in their wells, with identical confinement in each direction. Atomic wavefunctions can then be approximated by harmonic oscillator ground states of variance parameter $\sigma = \sqrt{\hbar/(m\omega)}$ [30], where ω is the corresponding harmonic frequency. As will be clear shortly, σ acts as a natural cutoff parameter, quenching the coupling with high-frequency modes.

Specifically, we consider ^{23}Na impurity atoms trapped in a far-detuned optical lattice and a ^{87}Rb condensate. The condensate density is $n_0 = 10^{20}$ m^{-3}, the lattice wavelength is $\lambda = 600$ nm, and we have taken $2L = \lambda/2$ and $D = 2L$. The depth of the optical lattice is described by the parameter $\alpha \equiv V_0/E_{\mathrm{R}}$, V_0 being the optical lattice potential maximum intensity and $E_{\mathrm{R}} = \hbar^2 k^2/(2m)$ the recoil energy of impurity atoms in the lattice; in our evaluations we put $\alpha = 20$. Finally, we assume $a_{\mathrm{AB}} = 55a_0$ [31], where a_0 is the Bohr radius, for the scattering length of impurities–condensate mixtures. This parameter can be modified in laboratory with the help of Feshbach resonances.

4.1. Single impurity decoherence

We first examine the decoherence exponent of a single impurity

$$\Gamma_0(t) \equiv \Gamma_{\{0\},\{1\}}(t) \equiv \hbar^2 \sum_{\mathbf{k}} \frac{\left(1 - \cos \frac{E_{\mathbf{k}}}{\hbar} t\right)}{E_{\mathbf{k}}^2} \coth \frac{\beta E_{\mathbf{k}}}{2} \left| \Omega_{\mathrm{R},\mathbf{k}}^1 - \Omega_{\mathrm{L},\mathbf{k}}^1 \right|^2. \tag{27}$$

This quantity, which will be a useful benchmark in our analysis of the collective decoherence of impurity pairs, already shows interesting features. Assuming, from now on, that the condensate is at temperature $T = 0$, we obtain

$$\Gamma_0(t) = 8g_{\mathrm{AB}}^2 n_0 \sum_{\mathbf{k}} (|u_{\mathbf{k}}| - |v_{\mathbf{k}}|)^2 \, \mathrm{e}^{-k^2\sigma^2/2} \frac{\sin^2 \frac{E_{\mathbf{k}}}{2\hbar} t}{E_{\mathbf{k}}^2} \sin^2 (\mathbf{k} \cdot \mathbf{L}) . \tag{28}$$
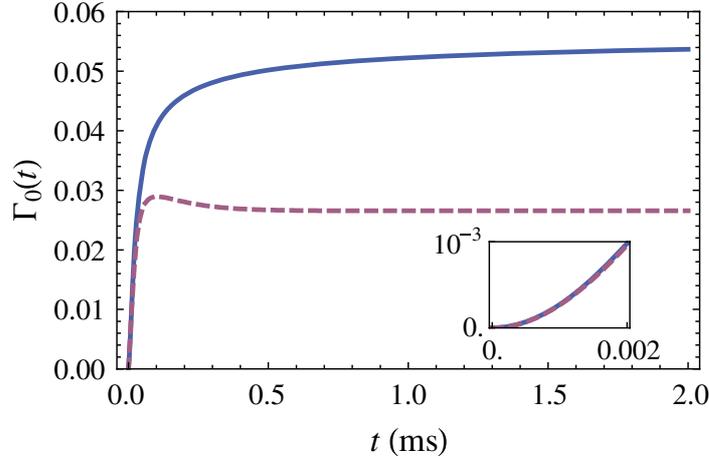
Figure 2. $\Gamma_0(t)$ versus time for a single impurity atom interacting with free bosons (solid line) and with a bosonic condensate (dashed line) in three dimensions. The inset shows $\Gamma_0(t)$ for very short times $0 \leqslant t \leqslant 2\,\mu$s.

We note the dependence of $\Gamma_0(t)$ on the length **L**, where 2**L** is the distance between two wells within each site. The presence of the factor $\sin^2(\mathbf{k} \cdot \mathbf{L})$ supresses the effect of the reservoir modes at small **k**. This is clearly understandable: environment modes whose wavelength is longer than **L** cannot 'resolve' the spatially separated wells within each site. The consequences of this fact will be clear shortly. Replacing the sum over discrete modes to a continuum with the usual rule $V^{-1} \sum_{\mathbf{k}} \to (2\pi)^{-3} \int d\mathbf{k}$, choosing x as azimuthal axis and using well-known relations for Bogoliubov modes [32], we finally obtain

$$\Gamma_0^c(t) = \frac{2g_{AB}^2 n_0}{\pi^2} \int_0^\infty dk \left[k^2 e^{-k^2\sigma^2/2} \frac{\sin^2 \frac{E_{\mathbf{k}}}{2\hbar}t}{E_{\mathbf{k}}(\epsilon_{\mathbf{k}} + 2g_B n_0)} \right] \left(1 - \frac{\sin 2kL}{2kL} \right). \qquad (29)$$

The superscript c is to remind us that we are dealing with impurities interacting with a condensate. For the special case of a bath of non-interacting bosons $\Gamma_0^{n.i.}(t)$ is obtained from (29) simply imposing $g_B = 0$ and $E_{\mathbf{k}} = \epsilon_{\mathbf{k}}$. Let us point out that the spectral density, which reads

$$J(\omega) \equiv \sum_{\mathbf{k}} |\Omega_{R,\mathbf{k}} - \Omega_{L,\mathbf{k}}|^2 \delta(\hbar\omega - E_{\mathbf{k}}), \qquad (30)$$

has a nontrivial form, which at small frequencies, scales as ω^{d+2} for the interacting case, where d is the dimensionality of the condensate, and as $\omega^{d/2}$ for the non-interacting case. It is worth noticing that while the former case is always superohmic, the latter is subohmic, ohmic and superohmic depending on the dimensionality of the environment. Note that the high power in $J(\omega)$ is due to the fact that the bath has to 'resolve' the structure of the impurity, formally again the factor $\sin^2(\mathbf{k} \cdot \mathbf{L})$. Furthermore, as already pointed out, no *ad hoc* cutoff frequency ω_c needs to be inserted but appears naturally in the decaying exponential of variance σ in (29).

Figure 2 shows clearly that the impurity maintains much of its coherence at long times. Such survival is due to the above-mentioned suppressed effect of soft modes, which are

responsible for the long time behaviour of $\Gamma_0(t)$, and is more pronounced when the environment consists of a condensate than in the case of a reservoir consisting of free bosons. This can be intuitively described in terms of greater 'stiffness' of the condensate whose Bogoliubov modes are less displaced by the coupled impurity. The condensate is even able to give some coherence back to the impurity, since $\Gamma_0^c(t)$ is not monotonic in time. Oscillations of coherence in spin-boson systems were predicted in [24] (and even earlier, in a different context, in [33]).

We can distinguish three stages in the dynamics of the Γ_0. In the first stage $\Gamma_0(t) \propto t^2$, as can be easily seen from a series expansion of (29). This very short stage, shown in the inset of figure 2, corresponds to coherent dynamics. The second stage corresponds to a Markovian behaviour, i.e. $\Gamma_0(t) \propto t$, and lasts a few tens of microseconds. Finally, in the third stage $\Gamma_0(t)$ saturates to a stationary value. This behaviour calls for particular caution in treating an environment of (free or interacting) bosons as a Markovian reservoir for atomic impurities immersed in it, which is clearly not the case in the present situation.

4.2. Collective decoherence of two impurities

Decoherence of quantum systems in a common environment is characterized by collective decoherence. It is well known that two spins interacting with the same bosonic reservoir with a spin-boson interaction Hamiltonian like the one discussed in this paper show sub- and superdecoherence [23]. Put simply, the decoherence rate of the two spins is not simply $2\Gamma_0(t)$ but, according to the initial state of the spins, much smaller or larger. In this final section of the present paper, we analyse the specific features of collective decoherence in our system.

For two pseudospins, three decoherence parameters appear in the density matrix elements independently of the exact form of the impurities' state. One is $\Gamma_0(t)$ and appears in elements such as $\rho_{0,0;0,1}(t)$, $\rho_{0,1;1,1}(t)$, etc which corresponds to individual dephasing of each impurity atom; two more parameters $\Gamma_1(t)$ and $\Gamma_2(t)$ appear in elements such as $|\rho_{0,0;1,1}(t)| = \exp[-\Gamma_1(t)]|\rho_{0,0;1,1}(0)|$ and $|\rho_{0,1;1,0}(t)| = \exp[-\Gamma_2(t)]|\rho_{0,1;1,0}(0)|$, and corresponds to decay of the coherences between states with the particles in the same or in the opposite side, respectively, of the double well. For two pseudospins at distance $2\mathbf{D} = 4L$, these two parameters are

$$\Gamma_1(t) \equiv \Gamma_{\{0,0\},\{1,1\}}(t) = \hbar^2 \sum_{\mathbf{k}} \frac{\left(1 - \cos\frac{E_{\mathbf{k}}}{\hbar}t\right)}{E_{\mathbf{k}}^2} \coth\frac{\beta E_{\mathbf{k}}}{2} \left|\left(\Omega_{R,\mathbf{k}}^1 - \Omega_{L,\mathbf{k}}^1 + \Omega_{R,\mathbf{k}}^2 - \Omega_{L,\mathbf{k}}^2\right)\right|^2$$

$$= 32g_{AB}^2 n_0 \sum_{\mathbf{k}} (|u_{\mathbf{k}}| - |v_{\mathbf{k}}|)^2 \, e^{-k^2\sigma^2/2} \frac{\sin^2\frac{E_{\mathbf{k}}}{2\hbar}t}{E_{\mathbf{k}}^2} \sin^2(\mathbf{k}\cdot\mathbf{L}) \cos^2(\mathbf{k}\cdot\mathbf{D}), \tag{31}$$

$$\Gamma_2(t) \equiv \Gamma_{\{1,0\},\{0,1\}}(t) = \hbar^2 \sum_{\mathbf{k}} \frac{\left(1 - \cos\frac{E_{\mathbf{k}}}{\hbar}t\right)}{E_{\mathbf{k}}^2} \coth\frac{\beta E_{\mathbf{k}}}{2} \left|\left(\Omega_{R,\mathbf{k}}^1 - \Omega_{L,\mathbf{k}}^1 - \Omega_{R,\mathbf{k}}^2 + \Omega_{L,\mathbf{k}}^2\right)\right|^2$$

$$= 32g_{AB}^2 n_0 \sum_{\mathbf{k}} (|u_{\mathbf{k}}| - |v_{\mathbf{k}}|)^2 \, e^{-k^2\sigma^2/2} \frac{\sin^2\frac{E_{\mathbf{k}}}{2\hbar}t}{E_{\mathbf{k}}^2} \sin^2(\mathbf{k}\cdot\mathbf{L}) \sin^2(\mathbf{k}\cdot\mathbf{D}). \tag{32}$$

Figure 3. $\Gamma_1(t)$ (dashed line), $\Gamma_2(t)$ (dotted line), and $2\Gamma_0(t)$ (solid line) versus time for a pair of impurity atoms at a distance $2D = 4L$ (see text), immersed in a condensate (left) and in an environment of free bosons (right) in three dimensions.

Calculations similar to those performed for Γ_0 give for a condensate environment

$$\Gamma_1^c(t) = \frac{2g_{AB}^2 n_0}{\pi^2} \int_0^\infty dk\, k^2 e^{-k^2\sigma^2/2} \frac{\sin^2\frac{E_k}{2\hbar}t}{E_k\,(\epsilon_k + 2g_B n_0)}$$

$$\times \left(2 - 2\frac{\sin 2kL}{2kL} + 2\frac{\sin 2kD}{2kD} - \frac{\sin 2k(L+D)}{2k(L+D)} - \frac{\sin 2k(D-L)}{2k(D-L)} \right)$$

$$\equiv 2\Gamma_0(t) - \delta^c(t), \tag{33}$$

$$\Gamma_2^c(t) = \frac{2g_{AB}^2 n_0}{\pi^2} \int_0^\infty dk\, k^2 e^{-k^2\sigma^2/2} \frac{\sin^2\frac{E_k}{2\hbar}t}{E_k\,(\epsilon_k + 2g_B n_0)}$$

$$\times \left(2 - 2\frac{\sin 2kL}{2kL} - 2\frac{\sin 2kD}{2kD} + \frac{\sin 2k(L+D)}{2k(L+D)} + \frac{\sin 2k(D-L)}{2k(D-L)} \right)$$

$$\equiv 2\Gamma_0(t) + \delta^c(t). \tag{34}$$

In the above equations, it is easy to identify the term $\delta^c(t)$ which quantifies the deviation to the dechoherence exponent $2\Gamma_0$ typical of the decoherence of two impurities interacting with independent environments. Note that while Γ_0 depends only on **L**, i.e. on the spatial size of the double well, δ depends nontrivially on $\mathbf{L} \pm \mathbf{D}$, i.e. on the distance between the impurities of different wells. As before the special case of a bath of non-interacting bosons $\Gamma_1^{n.i}(t)$, $\Gamma_2^{n.i\cdot}(t)$ are obtained from the above equations (33) simply imposing $g_B = 0$ and $E_k = \epsilon_k$.

As in the case of single impurity decoherence the impurities do not loose all their coherence: Γ_1 and Γ_2 saturate to a stationary value that can be varied with the help of Feshbach resonances. Furthermore figure 3 shows that in a system of two impurities coherence oscillations appear, both for interacting and non-interacting bosons in the environment (even more pronounced oscillation are shown in figure 5). Such coherence revival is due to the collective nature of the coupling, as quantified by $\delta^c(t)$ ($\delta^{n.i\cdot}(t)$ for free bosons). As shown
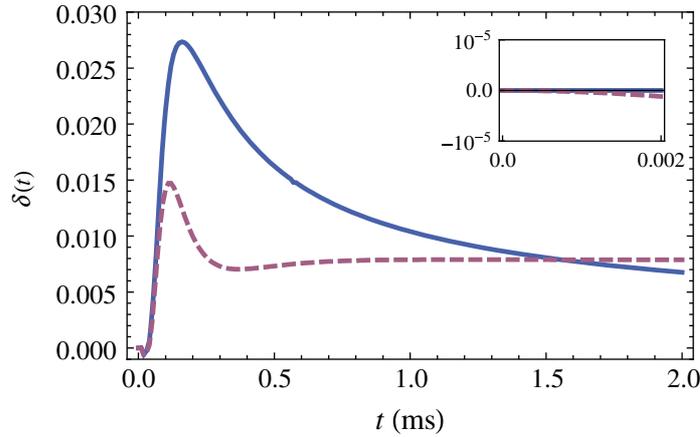
Figure 4. $\delta^c(t)$ (dashed line) and $\delta^{n.i.}(t)$ (solid line) versus time for a pair of impurity atoms in a 3D environment. The inset shows $\delta(t)$ for very short times $0 \leqslant t \leqslant 2\,\mu\text{s}$.

in figure 4 also the $\delta(t)$ are characterized by three different timescales comparable to those analysed for $\Gamma_0(t)$. In the first stage, the difference $|\delta(t)|$ is negligible, since the presence of each impurity cannot have modified yet the environment seen by the other one; in the second stage, corresponding to the Markovian dynamics, the difference $|\delta(t)|$ steadily grows up; and in the third stage it decreases, reaching a stationary value.

For a pair of impurities we observe super- and sub-decoherences; however, with a peculiarity which is characteristic of the system here considered. Indeed we observe sub-decoherence in $\Gamma_1 \equiv \Gamma_{\{0,0\},\{1,1\}}$ and super-decoherence with $\Gamma_2 \equiv \Gamma_{\{1,0\},\{0,1\}}$, at variance with what one observes in a standard spin-boson model, where their role would be exchanged [23]. This different behaviour is due to the particular configuration of our system: Γ_1 gets contribution from superpositions of the states $|0,0\rangle$ and $|1,1\rangle$, where the atoms sit in wells with identical distance, whereas the states $|0,1\rangle$ and $|1,0\rangle$, contributing to Γ_2, correspond to atoms sitting in wells with different separations.

Further insight on the features of the collective decoherence is gained by considering the decoherence of impurities sitting in sites which are at a larger distance than $2D = 4L = 600\,\text{nm}$. In figure 5, we plot the decoherence exponents for impurities trapped in lattice sites at distances $2D = 8L$, $16L$ and $40L$, respectively. These plots suggest the following picture: initially the impurities decohere independently, as if they were each immersed in its own environment; at some later time, the environment correlations due to the impurities act back on them and give rise to oscillating deviations from $2\Gamma_0(t)$. The onset time of these oscillations depends on the separation: the larger the separation, the later the onset. On the other hand, the correlations become weaker as the distance increases and the oscillations become consequently smaller in amplitude. At large separation (here, approximately $40L$), the parameters Γ_1 and Γ_2 are hardly discernible from $2\Gamma_0$, since the environment correlations induced by the impurities vanish. Similar features in a related context are reported in [34]. In summary, $\Gamma_1(t)$ and $\Gamma_2(t)$ also prompt information about the correlation length of the environment.
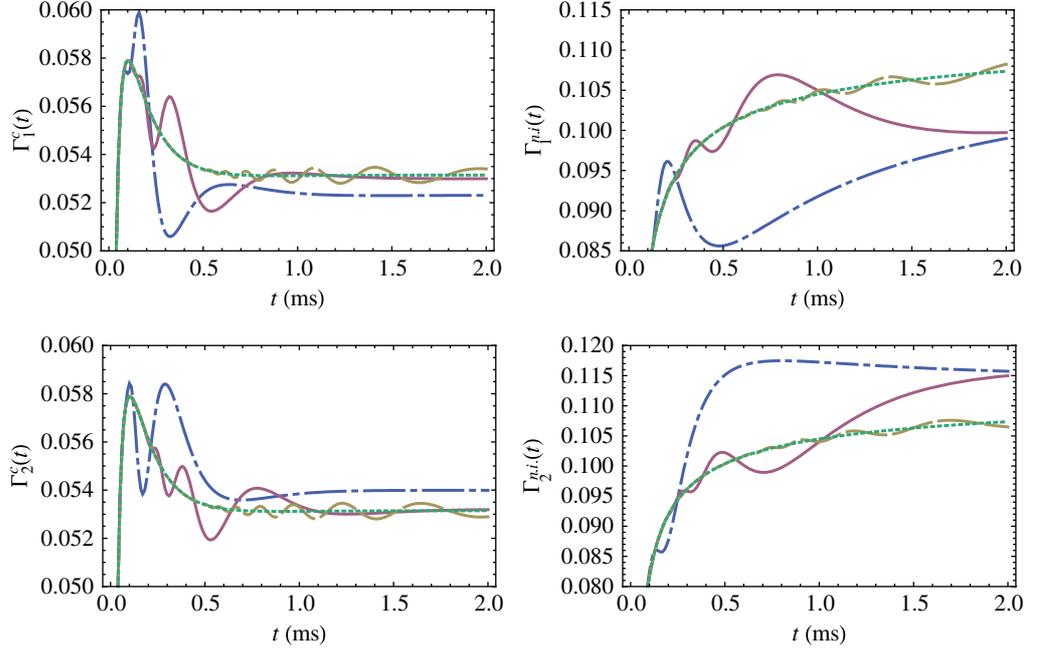
Figure 5. $\Gamma_1(t)$ (top) and $\Gamma_2(t)$ (bottom) versus time for a pair of impurity atoms interacting with a bosonic condensate (left) and with free bosons (right) in three dimensions for different distances between the impurities: $2D = 8L$ (dash-dotted line), $2D = 16L$ (solid line), and $2D = 40L$ (dashed line); $2\Gamma_0(t)$ (dotted line) is also shown for comparison.

4.3. Decoherence in one dimension

Finally, we examine the decoherence process in a 1D condensate. Since, as previously discussed, the spectral density (30) is superohmic for an interacting gas, but subohmic for a free Bose gas, we expect qualitative different results for the two cases, in contrast to the 3D case. The decay exponents in one dimension $\gamma(t)$ become

$$\gamma_0^c(t) = \frac{4g_{AB}^2 n_0}{\pi} \int_{-\infty}^{\infty} dk \left[e^{-k^2\sigma^2/2} \frac{\sin^2 \frac{E_\mathbf{k}}{2\hbar}t}{E_\mathbf{k}(\epsilon_\mathbf{k} + 2g_B n_0)} \right] \sin^2 kL \tag{35}$$

for one impurity and

$$\gamma_1^c(t) = \frac{4g_{AB}^2 n_0}{\pi} \int_{-\infty}^{\infty} dk \left[e^{-k^2\sigma^2/2} \frac{\sin^2 \frac{E_\mathbf{k}}{2\hbar}t}{E_\mathbf{k}(\epsilon_\mathbf{k} + 2g_B n_0)} \right] \sin^2(kL) \cos^2(kD)$$

$$\equiv 2\gamma_0(t) - \delta^c(t), \tag{36}$$

$$\gamma_2^c(t) = \frac{4g_{AB}^2 n_0}{\pi} \int_{-\infty}^{\infty} dk \left[e^{-k^2\sigma^2/2} \frac{\sin^2 \frac{E_\mathbf{k}}{2\hbar}t}{E_\mathbf{k}(\epsilon_\mathbf{k} + 2g_B n_0)} \right] \sin^2(kL) \sin^2(kD)$$

$$\equiv 2\gamma_0(t) + \delta^c(t) \tag{37}$$

for two impurities in a condensate. The behaviour of these parameters critically depends on the nature of the environment, see figure 6. In particular, decoherence in a 1D sample of free bosons
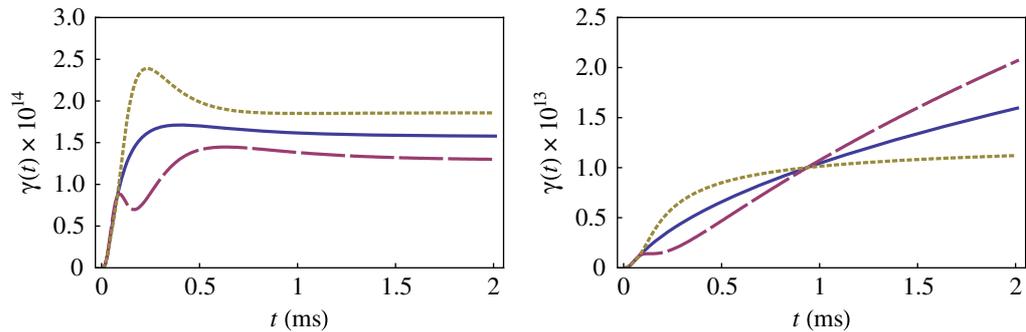
Figure 6. $\gamma_1(t)$ (dashed line), $\gamma_2(t)$ (dotted line), and $2\gamma_0(t)$ (solid line) versus time for a pair of impurity atoms immersed in a condensate (left) and in an environment of free bosons (right) in one dimension. The separation between two impurity atoms is $2D = 4L$.

becomes Markovian, in agreement with the naive expectation, due to its subohmic spectral density.

5. Conclusions

We have shown how a system of impurity atoms trapped in an array of double wells, interacting with a cold atomic gas, is described, in a suitable regime, by a spin-boson Hamiltonian. The specific nature of our system, in which the pseudospins associated with the presence of an impurity in the right/left well of each site have a spatial dimension, introduces peculiar features in the decoherence of a single impurity as well as in the collective decoherence, with the persistence of coherence at long times, the presence of coherence oscillations and counterintuitive super/subdecoherent states.

We have shown in particular that for a three-dimensional bath one never has a Markovian behaviour. A 1D bath is in this respect more interesting since one can go from a non-Markovian to a Markovian behaviour just by tuning the interaction of the bath.

As a final comment we would like to say a few words about the role of the quadratic terms in the Bogoliubov operators which we have neglected in our derivation of Hamiltonian (14). Although a detailed study of their effects is beyond the scope of the present paper, we would like to point out that their effects are negligible with respect to the linear terms we have analysed here. One can show that their inclusion amounts to taking into account elastic scattering of Bogoliubov particles, which is simply responsible of an energy shift, inelastic scattering processes and Bogoliubov pair creation and annihilation. In these two latter additional terms the length of wave vectors k that can play some role in the impurities' dynamics is limited from below by the finite size of the condensate and from above by cutoff parameter σ^{-1}. It can be shown that, in this frequency range, the coupling constants of the neglected processes are, for the values of parameters assumed in our analysis, three orders of magnitude smaller than the coupling constants $\hbar\Omega_{n,\mathbf{k}}^i$ of the linear terms. As a consequence, a rough estimate leads us to suppose that any possible relevant effect of the quadratic terms in the Hamiltonian would become apparent at timescales that are three orders of magnitude larger than those examined in this paper.

Acknowledgments

Appendix A. Disentangling the time-evolution operator

The factorization of the time-evolution operator $\hat{U}(t) = \exp[-i\hat{H}t/\hbar]$ is often an impossible task. When the Hamiltonian contains operators forming a Lie algebra the transformation of $\hat{U}(t)$ into a product of simpler exponential operators is however possible in some cases [35]. Here, we show a practical way to transform $\hat{U}(t)$, which we write as

$$\hat{U}(t) = \exp\left[-\frac{i}{\hbar}\sum_{\mathbf{k}} E_{\mathbf{k}}\hat{c}_{\mathbf{k}}^{\dagger}\hat{c}_{\mathbf{k}}t\right]\exp\left[\sum_{\mathbf{k}}\left(\sum_{i} A_{\mathbf{k}}^{i}(t)\hat{\sigma}_{z}^{i} + \alpha_{\mathbf{k}}(t)\right)\hat{c}_{\mathbf{k}}^{\dagger}\right]$$
$$\times \exp\left[-\sum_{\mathbf{k}}\left(\sum_{i} B_{\mathbf{k}}^{i}(t)\hat{\sigma}_{z}^{i} + \beta_{\mathbf{k}}(t)\right)\hat{c}_{\mathbf{k}}\right]\hat{U}_{\mathrm{R}}(t), \tag{A.1}$$

where $\hat{U}_{\mathrm{R}}(t)$ is to be determined, as well as the quantities $A_{\mathbf{k}}^{i}(t)$, $B_{\mathbf{k}}^{i}(t)$, $\alpha_{\mathbf{k}}(t)$ and $\beta_{\mathbf{k}}(t)$. Since at $t = 0$ the time-evolution operator $\hat{U}$ reduces to the identity operator, $A_{\mathbf{k}}^{i}(0) = B_{\mathbf{k}}^{i}(0) = \beta_{\mathbf{k}}(0) = \alpha_{\mathbf{k}}(0) = 0$. All unknown quantities can be found with the help of the relation

$$\hat{H} = i\hbar\left[d\hat{U}(t)/dt\right]\hat{U}^{-1}(t), \tag{A.2}$$

which holds for any time-independent Hamiltonian and of the relation

$$e^{\hat{X}}\hat{Y}e^{-\hat{X}} = \hat{Y} + [\hat{X}, \hat{Y}] + \tfrac{1}{2}[\hat{X}, [\hat{X}, \hat{Y}]] + \tfrac{1}{6}[\hat{X}, [\hat{X}, [\hat{X}, \hat{Y}]]] + \cdots \tag{A.3}$$

for arbitrary operators $\hat{X}$ and $\hat{Y}$. After inserting the expression (A.1) for the time-evolution operator $\hat{U}(t)$ in the right-hand side of (A.2), a comparison with the Hamiltonian (18) leads to the expressions

$$A_{\mathbf{k}}^{i}(t) = \frac{\hbar\left(\Omega_{\mathrm{R},\mathbf{k}}^{i*} - \Omega_{\mathrm{L},\mathbf{k}}^{i*}\right)}{2E_{\mathbf{k}}}\left(1 - e^{iE_{\mathbf{k}}t/\hbar}\right), \quad B_{\mathbf{k}}^{i}(t) = A_{\mathbf{k}}^{i*}(t), \tag{A.4}$$

$$\alpha_{\mathbf{k}}(t) = \frac{\hbar\sum_{i}\left(\Omega_{\mathrm{R},\mathbf{k}}^{i*} + \Omega_{\mathrm{L},\mathbf{k}}^{i*}\right)}{2E_{\mathbf{k}}}\left(1 - e^{iE_{\mathbf{k}}t/\hbar}\right), \quad \beta_{\mathbf{k}}(t) = \alpha_{\mathbf{k}}^{*}(t) \tag{A.5}$$

for $A(t)$, $B(t)$, $\alpha(t)$ and $\beta(t)$, and to the differential equation

$$\frac{d}{dt}\hat{U}_{\mathrm{R}}(t) = -\sum_{\mathbf{k}}\left(\sum_{i}\dot{B}_{\mathbf{k}}^{i}(t)\hat{\sigma}_{z}^{i} + \dot{\beta}_{\mathbf{k}}(t)\right)\left(\sum_{j}A_{\mathbf{k}}^{j}(t)\hat{\sigma}_{z}^{j} + \alpha_{\mathbf{k}}(t)\right)\hat{U}_{\mathrm{R}}(t) \tag{A.6}$$

for the unknown exponential operator $\hat{U}_{\mathrm{R}}(t)$, which we write as

$$\hat{U}_{\mathrm{R}}(t) = \exp\left[-\sum_{\mathbf{k}}\left(\sum_{ij}\eta_{\mathbf{k}}^{ij}(t)\hat{\sigma}_{z}^{i}\hat{\sigma}_{z}^{j} + \sum_{i}\mu_{\mathbf{k}}^{i}(t)\hat{\sigma}_{z}^{i} + \epsilon_{\mathbf{k}}(t)\right)\right]. \tag{A.7}$$

A comparison with (A.6) gives

$$\dot{\eta}_{\mathbf{k}}^{ij}(t) = \dot{B}_{\mathbf{k}}^i(t) A_{\mathbf{k}}^j(t), \quad \dot{\epsilon}_{\mathbf{k}}(t) = \dot{\beta}_{\mathbf{k}}(t)\alpha_{\mathbf{k}}(t), \quad \dot{\mu}_{\mathbf{k}}^i(t) = \dot{B}_{\mathbf{k}}^i(t)\alpha_{\mathbf{k}}(t) + \dot{\beta}_{\mathbf{k}}(t) A_{\mathbf{k}}^i(t) \tag{A.8}$$

that is

$$\eta_{\mathbf{k}}^{ij}(t) = -\mathrm{i}\hbar \frac{(\Omega_{\mathrm{R,\mathbf{k}}}^i - \Omega_{\mathrm{L,\mathbf{k}}}^i)\left(\Omega_{\mathrm{R,\mathbf{k}}}^{j*} - \Omega_{\mathrm{L,\mathbf{k}}}^{j*}\right)}{4E_{\mathbf{k}}}\left[t + \frac{\mathrm{i}\hbar}{E_{\mathbf{k}}}\left(1 - \mathrm{e}^{-\mathrm{i}E_{\mathbf{k}}t/\hbar}\right)\right], \tag{A.9}$$

$$\epsilon_{\mathbf{k}}(t) = -\mathrm{i}\hbar \frac{\sum_{ij}(\Omega_{\mathrm{R,\mathbf{k}}}^i + \Omega_{\mathrm{L,\mathbf{k}}}^i)\left(\Omega_{\mathrm{R,\mathbf{k}}}^{j*} + \Omega_{\mathrm{L,\mathbf{k}}}^{j*}\right)}{4E_{\mathbf{k}}}\left[t + \frac{\mathrm{i}\hbar}{E_{\mathbf{k}}}\left(1 - \mathrm{e}^{-\mathrm{i}E_{\mathbf{k}}t/\hbar}\right)\right], \tag{A.10}$$

$$\mu_{\mathbf{k}}^i(t) = -\frac{\mathrm{i}\hbar}{2E_{\mathbf{k}}}\Re\left[(\Omega_{\mathrm{R,\mathbf{k}}}^i - \Omega_{\mathrm{L,\mathbf{k}}}^i)\sum_j\left(\Omega_{\mathrm{R,\mathbf{k}}}^{j*} + \Omega_{\mathrm{L,\mathbf{k}}}^{j*}\right)\right]\left[t + \frac{\mathrm{i}\hbar}{E_{\mathbf{k}}}\left(1 - \mathrm{e}^{-\mathrm{i}E_{\mathbf{k}}t/\hbar}\right)\right]. \tag{A.11}$$

Moreover, using Glauber's relation

$$\exp\left[\sum_{\mathbf{k}} g_{\mathbf{k}}\hat{c}_{\mathbf{k}}^\dagger\right]\exp\left[-\sum_{\mathbf{k}} g_{\mathbf{k}}^*\hat{c}_{\mathbf{k}}\right] = \exp\left[\sum_{\mathbf{k}}\left(g_{\mathbf{k}}\hat{c}_{\mathbf{k}}^\dagger - g_{\mathbf{k}}^*\hat{c}_{\mathbf{k}}\right)\right]\exp\left[\frac{1}{2}\sum_{\mathbf{k}}|g_{\mathbf{k}}|^2\right] \tag{A.12}$$

the two exponentials linear in Bogoliubov operators can be merged into

$$\exp\left[\sum_{\mathbf{k}}\left(\sum_i A_{\mathbf{k}}^i(t)\hat{\sigma}_z^i + \alpha_{\mathbf{k}}(t)\right)\hat{c}_{\mathbf{k}}^\dagger\right]\exp\left[-\sum_{\mathbf{k}}\left(\sum_i B_{\mathbf{k}}^i(t)\hat{\sigma}_z^i + \beta_{\mathbf{k}}(t)\right)\hat{c}_{\mathbf{k}}\right]$$

$$= \exp\left\{\left[\sum_{\mathbf{k}}\left(\sum_i A_{\mathbf{k}}^i(t)\hat{\sigma}_z^i + \alpha_{\mathbf{k}}(t)\right)\hat{c}_{\mathbf{k}}^\dagger - \sum_{\mathbf{k}}\left(\sum_i A_{\mathbf{k}}^{i*}(t)\hat{\sigma}_z^i + \alpha_{\mathbf{k}}^*(t)\right)\hat{c}_{\mathbf{k}}\right]\right\}$$

$$\times \exp\left\{\frac{1}{2}\left[\sum_{\mathbf{k}}\left(\sum_i A_{\mathbf{k}}^i(t)\hat{\sigma}_z^i + \alpha_{\mathbf{k}}(t)\right)\left(\sum_j A_{\mathbf{k}}^{j*}(t)\hat{\sigma}_z^j + \alpha_{\mathbf{k}}^*(t)\right)\right]\right\} \tag{A.13}$$

and the contribution of the last exponential can be included in $U_R(t)$. Performing some commutations where it is possible, the time-evolution operator becomes

$$\hat{U}(t) = \exp\left[-\frac{\mathrm{i}}{\hbar}\sum_{\mathbf{k}} E_{\mathbf{k}}\hat{c}_{\mathbf{k}}^\dagger\hat{c}_{\mathbf{k}}t\right]\exp\left[-\sum_{\mathbf{k}}\left(\sum_{ij}\eta_{\mathbf{k}}^{ij}(t)\hat{\sigma}_z^i\hat{\sigma}_z^j + \sum_i \mu_{\mathbf{k}}^i(t)\hat{\sigma}_z^i + \epsilon_{\mathbf{k}}(t)\right)\right]$$

$$\times \exp\left[\sum_{\mathbf{k}}\left(\sum_i A_{\mathbf{k}}^i(t)\hat{\sigma}_z^i + \alpha_{\mathbf{k}}(t)\right)\hat{c}_{\mathbf{k}}^\dagger - \sum_{\mathbf{k}}\left(\sum_i B_{\mathbf{k}}^i(t)\hat{\sigma}_z^i + \beta_{\mathbf{k}}(t)\right)\hat{c}_{\mathbf{k}}\right]$$

$$\times \exp\left\{\frac{1}{2}\left[\sum_{\mathbf{k}}\left(\sum_i A_{\mathbf{k}}^i(t)\hat{\sigma}_z^i + \alpha_{\mathbf{k}}(t)\right)\left(\sum_j A_{\mathbf{k}}^{j*}(t)\hat{\sigma}_z^j + \alpha_{\mathbf{k}}^*(t)\right)\right]\right\}. \tag{A.14}$$

Finally, the exponential operators that do not contain bath operators commute, so the time-evolution operator can be further modified into the final form (19).

Appendix B. Derivation of the dynamics of the impurities

The action of $\hat{U}_{\mathbf{k},\mathrm{D}}(t)$ on a pure state of the whole system is

$$
\hat{U}_{\mathbf{k},\mathrm{D}}(t)|\{n_p\}\rangle\langle\{m_p\}|\otimes\rho_{\mathbf{k}}\hat{U}^{\dagger}_{\mathbf{k},\mathrm{D}}(t) = |\{n_p\}\rangle\langle\{m_p\}|\otimes
$$

$$
\times\exp\left[\left(-\sum_j A^j_{\mathbf{k}}(t)(-1)^{n_j}+\alpha_{\mathbf{k}}(t)\right)\hat{c}^{\dagger}_{\mathbf{k}} - \left(-\sum_j A^{j*}_{\mathbf{k}}(t)(-1)^{n_j}+\alpha^*_{\mathbf{k}}(t)\right)\hat{c}_{\mathbf{k}}\right]\rho_{\mathbf{k}}
$$

$$
\times\exp\left[-\left(-\sum_j A^j_{\mathbf{k}}(t)(-1)^{m_j}+\alpha_{\mathbf{k}}(t)\right)\hat{c}^{\dagger}_{\mathbf{k}} + \left(-\sum_j A^{j*}_{\mathbf{k}}(t)(-1)^{m_j}+\alpha^*_{\mathbf{k}}(t)\right)\hat{c}_{\mathbf{k}}\right]
$$

(B.1)

and the density matrix elements $\rho_{\{n_p\},\{m_p\}}(t)$ of the impurities are obtained by tracing over the bath,

$$
\rho_{\{n_p\},\{m_p\}}(t) = \exp\left\{i\Theta_{\{n_p\},\{m_p\}}(t)\right\}\exp\left\{i\Xi_{\{n_p\},\{m_p\}}(t)\right\}\rho_{\{n_p\},\{m_p\}}(0)
$$

$$
\times\langle\{n_p\}|\prod_{\mathbf{k}}\mathrm{Tr}_{\mathrm{B},\mathbf{k}}\left\{\hat{U}_{\mathbf{k},\mathrm{D}}(t)|\{n_p\}\rangle\langle\{m_p\}|\otimes\rho_{\mathbf{k}}\hat{U}^{\dagger}_{\mathbf{k},\mathrm{D}}(t)\right\}|\{m_p\}\rangle,
$$

(B.2)

where $\mathrm{Tr}_{\mathrm{B},\mathbf{k}}$ denotes the trace over each Bogoliubov mode of the environment and the phases

$$
\Theta_{\{n_p\},\{m_p\}}(t) = \hbar^2\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}(t)}{4E^2_{\mathbf{k}}}\sum_{ij}\Re\left(\Omega^i_{\mathrm{R},\mathbf{k}}-\Omega^i_{\mathrm{L},\mathbf{k}}\right)\left(\Omega^{j*}_{\mathrm{R},\mathbf{k}}-\Omega^{j*}_{\mathrm{L},\mathbf{k}}\right)\left[(-1)^{n_i+n_j}-(-1)^{m_i+m_j}\right],\quad\text{(B.3)}
$$

$$
\Xi_{\{n_p\},\{m_p\}}(t) = \hbar^2\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}(t)}{E^2_{\mathbf{k}}}\Re\sum_j\left(\Omega^{j*}_{\mathrm{R},\mathbf{k}}+\Omega^{j*}_{\mathrm{L},\mathbf{k}}\right)\sum_i\left(\Omega^i_{\mathrm{R},\mathbf{k}}-\Omega^i_{\mathrm{L},\mathbf{k}}\right)(n_i-m_i)\qquad\text{(B.4)}
$$

come from the unitary operators in (19). Performing cyclic permutation inside the trace and using the identity $\exp(\hat{M})\exp(\hat{N}) = \exp(\hat{M}+\hat{N})\exp[\hat{M},\hat{N}]/2$, which holds for operators $\hat{M}$ and $\hat{N}$ that commute with their commutator, the trace $\mathrm{Tr}_{\mathrm{B},\mathbf{k}}$ in (25) becomes

$$
\exp\left[i\Im\left(\sum_j A^j_{\mathbf{k}}(t)(-1)^{n_j}-\alpha_{\mathbf{k}}(t)\right)\left(\sum_j A^{j*}_{\mathbf{k}}(t)(-1)^{m_j}-\alpha^*_{\mathbf{k}}(t)\right)\right\}
$$

$$
\times\mathrm{Tr}_{\mathrm{B},\mathbf{k}}\left\{\exp\left[2\sum_i(n_i-m_i)\left(A^i_{\mathbf{k}}(t)\hat{c}^{\dagger}_{\mathbf{k}}-A^{i*}_{\mathbf{k}}(t)\hat{c}_{\mathbf{k}}\right)\right]\rho_{\mathbf{k}}\right\}
$$

$$
\equiv\exp\left\{i\Delta_{\{n_p\},\{m_p\}}(t)\right\}\mathrm{Tr}_{\mathrm{B},\mathbf{k}}\left\{\exp\left[2\sum_i(n_i-m_i)\left(A^i_{\mathbf{k}}(t)\hat{c}^{\dagger}_{\mathbf{k}}-A^{i*}_{\mathbf{k}}(t)\hat{c}_{\mathbf{k}}\right)\right]\rho_{\mathbf{k}}\right\}.
$$

(B.5)

The trace over the thermal bath of the displacement operators is well-known [23],

$$
\mathrm{Tr}_{\mathrm{B},\mathbf{k}}\left[\exp\left\{g_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}}-g^*_{\mathbf{k}}\hat{c}_{\mathbf{k}}\right\}\rho_{\mathbf{k}}\right] = \exp\left\{-\frac{|g_{\mathbf{k}}|^2}{2}\coth\frac{\beta E_{\mathbf{k}}}{2}\right\},\qquad\text{(B.6)}
$$

where $\beta = (k_{\mathrm{B}}T)^{-1}$, and leads to equation (25).

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Appendix C. The coupling constant in a deep optical lattice

In a deep optical lattice, the ground state wavefunctions of each well can be approximated with those of harmonic oscillators,

$$\varphi_{i,N}(\mathbf{x}) = \frac{1}{\left[\pi^3 x_0^2 y_0^2 z_0^2\right]^{1/4}} \exp\left[-\frac{(x - x_{i,N})^2}{2x_0^2} - \frac{(y - y_{i,N})^2}{2y_0^2} - \frac{(z - z_{i,N})^2}{2z_0^2}\right]. \tag{C.1}$$

Here $N = $ L, R, and $x_0 = \sqrt{\hbar/(m\omega_x)}$, $y_0 = \sqrt{\hbar/(m\omega_y)}$, and $z_0 = \sqrt{\hbar/(m\omega_z)}$, where the ω's are the trapping frequencies of the harmonic trap approximating the lattice potential at bottom of L and R wells of the lattice site i. The coupling frequencies (17) of the spin-boson model then become

$$\Omega_{n,\mathbf{k}}^i = \frac{g_{AB}\sqrt{n_0}}{\hbar}(|u_\mathbf{k}| - |v_\mathbf{k}|)\int \mathrm{d}^3x \, |\varphi_{i,L}(\mathbf{x})|^2 \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$$

$$= \frac{g_{AB}\sqrt{n_0}}{\hbar}(|u_\mathbf{k}| - |v_\mathbf{k}|)\,\mathrm{e}^{-k^2\sigma^2/4}\mathrm{e}^{\mathrm{i}k_x x_{i,n}}, \quad n = \mathrm{L, R} \tag{C.2}$$

having assumed identical confinement in the three directions, $\sigma = x_0 = y_0 = z_0$.

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Demons, Engines
and the Second Law

*Since 1871 physicists have been trying to resolve the conundrum
of Maxwell's demon: a creature that seems to violate the second law
of thermodynamics. An answer comes from the theory of computing*

by Charles H. Bennett

One manifestation of the second law of thermodynamics is that such devices as refrigerators, which create inequalities of temperature, require energy in order to operate. Conversely, an existing inequality of temperature can be exploited to do useful work—for example by a steam engine, which exploits the temperature difference between its hot boiler and its cold condenser. Yet in 1871 the Scottish physicist James Clerk Maxwell suggested, in his *Theory of Heat,* that a creature small enough to see and handle individual molecules might be exempt from this law. It might be able to create and sustain differences in temperature without doing any work:

"...if we conceive a being whose faculties are so sharpened that he can follow every molecule in its course, such a being, whose attributes are still as essentially finite as our own, would be able to do what is at present impossible to us. For we have seen that the molecules in a vessel full of air at uniform temperature are moving with velocities by no means uniform.... Now let us suppose that such a vessel is divided into two portions, A and B, by a division in which there is a small hole, and that a being, who can see the individual molecules, opens and closes this hole, so as to allow only the swifter molecules to pass from A to B, and only the slower ones to pass from B to A. He will thus, without expenditure of work, raise the temperature of B and lower that of A, in contradiction to the second law of thermodynamics."

The "being" soon came to be called Maxwell's demon, because of its far-reaching subversive effects on the natural order of things. Chief among these effects would be to abolish the need for energy sources such as oil, uranium and sunlight. Machines of all kinds could be operated without batteries, fuel tanks or power cords. For example, the demon would enable one to run a steam engine continuously without fuel, by keeping the engine's boiler perpetually hot and its condenser perpetually cold.

To protect the second law, physicists have proposed various reasons the demon cannot function as Maxwell described. Surprisingly, nearly all these proposals have been flawed. Often flaws arose because workers had been misled by advances in other fields of physics; many of them thought (incorrectly, as it turns out) that various limitations imposed by quantum theory invalidated Maxwell's demon.

The correct answer—the real reason Maxwell's demon cannot violate the second law—has been uncovered only recently. It is the unexpected result of a very different line of research: research on the energy requirements of computers.

Since Maxwell's day numerous versions of the demon have been proposed. One of the simplest creates a pressure difference (rather than a temperature difference) by allowing all molecules, fast or slow, to pass from B to A but preventing them from passing from A to B. Eventually most of the molecules will be concentrated in A and a partial vacuum will be created in B. This demon is if anything more plausible than Maxwell's original demon, since it would not need to be able to see or think. It is not immediately evident why such a demon—a one-way valve for molecules—could not be realized as some simple inanimate device, for instance a miniature spring-loaded trapdoor.

Like Maxwell's original demon, the "pressure demon" could be a source of limitless power for machines. For example, pneumatic drills of the kind used to cut holes in streets generally run on compressed air from a tank kept full by a gasoline-powered compressor. A one-way valve for air molecules could substitute for the compressor, effortlessly collecting air from the surroundings into the high-pressure tank.

One might think such an arrangement would violate the law of conservation of energy (otherwise known as the first law of thermodynamics), but it would not. The energy for cutting concrete could be taken from heat in the air collected by the one-way valve; the air's temperature would drop as it passed through the machinery. There is nothing in the first law to prevent an engine from supplying all its energy needs from the ambient heat of its environment, or even from the waste heat of its own friction and exhaust. It is the second law that prohibits such engines.

To analyze the demon's actions closely, then, one must understand some of the subtleties of the second law. The second law was originally expressed as a restriction on the possible transformations of heat and work, but it is now seen as being fundamentally a statement about the increase of disorder in the universe. According to the second law, the entropy, or disorder, of the universe as a whole cannot be made to decrease. This means that only two kinds of events are possible: events during which the entropy of the universe increases and events during which it remains constant. The former are
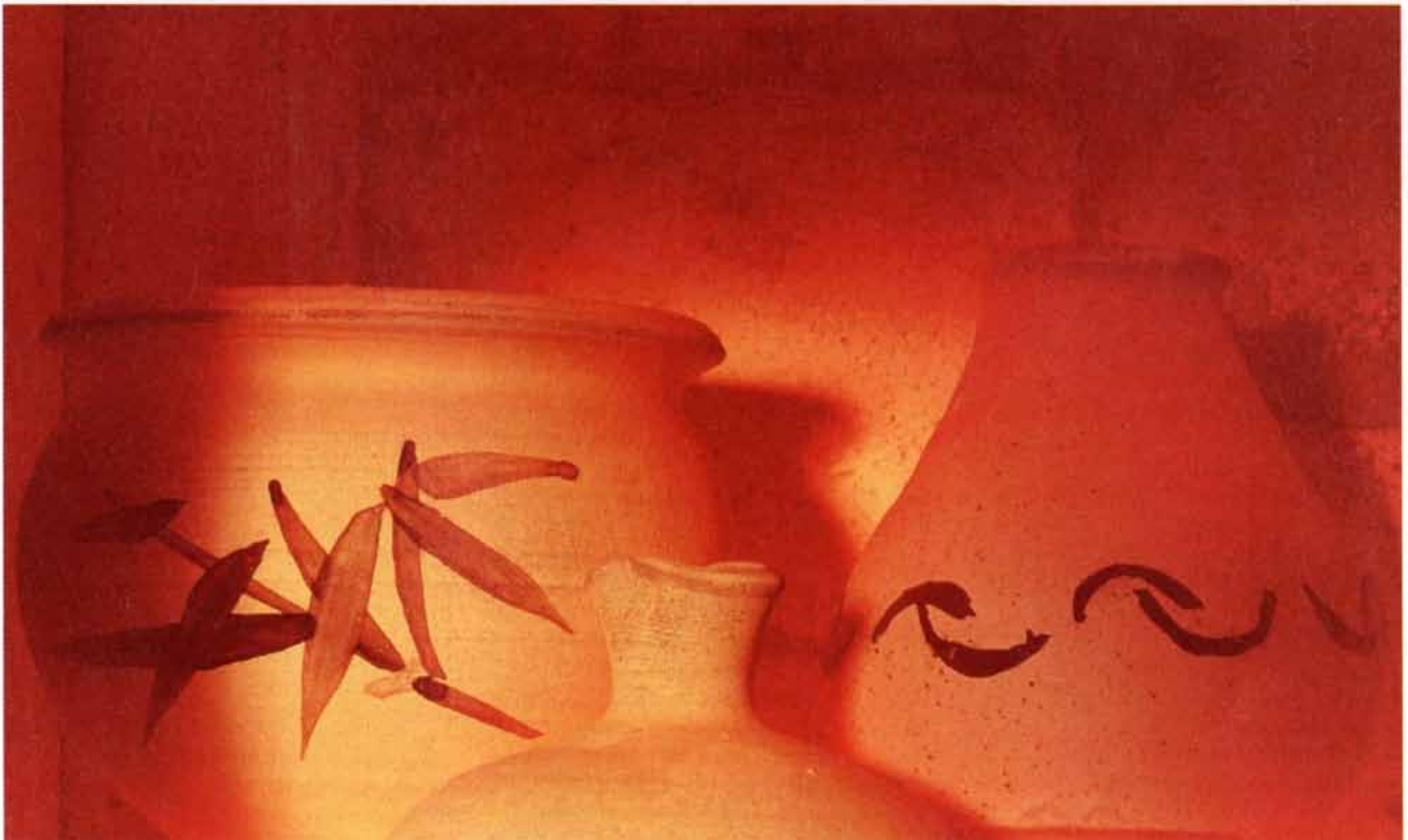
UNIFORM GLOW in a hot furnace (*top*) demonstrates one consequence of the second law of thermodynamics: it is impossible to distinguish objects in a vessel at uniform temperature without an external light source hotter than the vessel's ambient temperature. In a vessel at uniform temperature objects glow in such a way that exactly the same intensity and color of light come from the surface of every object (even objects that have different reflectances and colors). The reason is that if any object appeared darker than its surroundings, it would absorb energy at the expense of its neighbors. As a result it would become hotter and its neighbors would become cooler. According to the second law, however, objects that are initially at the same temperature cannot spontaneously come to have different temperatures. (In this photograph some contrast is visible because the temperature inside the furnace is not exactly uniform.) By an external light source, intrinsic differences in reflectance are visible (*bottom*).
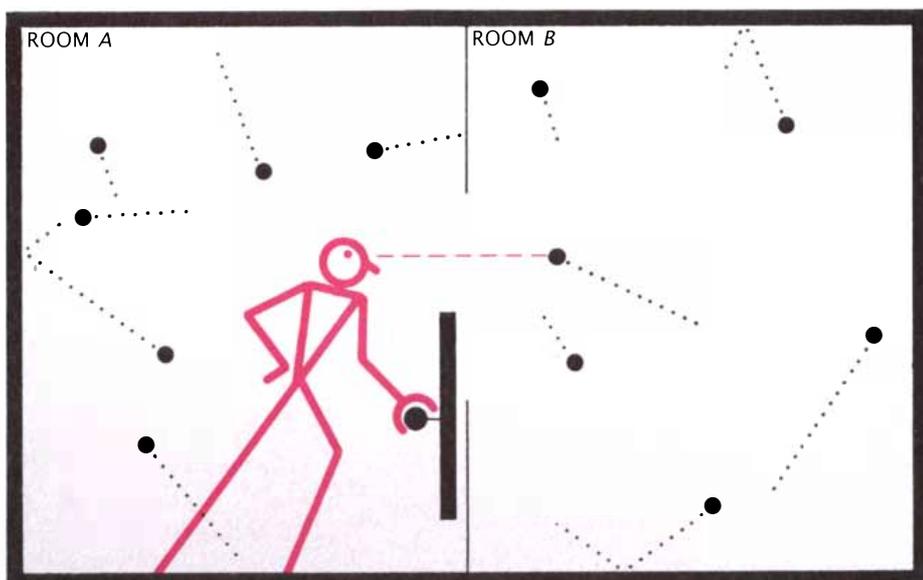
MAXWELL'S DEMON, described in 1871 by James Clerk Maxwell, seems able to violate the second law of thermodynamics. The demon controls a sliding door that blocks a hole in a wall between rooms containing gas at equal temperatures and pressures. It observes molecules approaching the hole and opens and closes the door to allow fast-moving molecules to pass from room A to room B but not vice versa. Slow-moving molecules, conversely, are allowed to pass only from B to A. As the demon sorts, B heats up and A cools. According to the second law, a certain amount of work is required to create a temperature difference, but the work of sliding a door can be made negligibly small.

known as irreversible processes because to undo them would violate the second law; the latter are called reversible processes. One can decrease the entropy of a given system by doing work on it, but in doing the work one would increase the entropy of another system (or that of the first system's environment) by an equal or greater amount.

A classic irreversible process, and one that helps in defining the concept of entropy a little more precisely, is called free expansion. Suppose a chamber filled with gas is separated by a partition from a vacuum chamber of the same size. If a small hole is made in the partition, gas will escape (that is, it will expand freely) into the formerly empty chamber until both chambers are filled equally.

The reason the molecules spread out to fill both chambers is mathematical rather than physical, if such a distinction can be made. The numbers of molecules on the two sides of the partition tend to equalize not because the molecules repel one another and move as far apart as possible, but rather because their many collisions with the walls of the container and with one another tend to distribute them randomly throughout the available space, until about half of them are on one side of the partition and about half are on the other side.

Since the spreading of the mole-cules is due to chance rather than to repulsion, there is a chance that all the molecules might return simultaneously to the chamber from which they came. If there are n molecules, however, the probability of all of them returning to their original chamber is the same as the probability of tossing n coins and having them all come up "heads": $1/2^n$. Thus for any sizable number of molecules (and there are about 300,000,000,-000,000,000,000,000 molecules in a gram of hydrogen) the free expansion is an effectively irreversible process: a process whose spontaneous undoing, although possible, is so unlikely that one can say with confidence it will never be observed.

The disordered state—the state in which the gas has spread into both chambers rather than residing compactly in a single chamber—is more probable than the ordered state. That is, there are more configurations of molecules in which the molecules occupy both chambers, just as, when 100 coins are tossed, there are more ways to achieve a total of 50 heads and 50 tails than there are to achieve 100 heads and no tails. In saying that the entropy of the universe tends to increase, the second law is simply noting that the universe tends to fall into more probable states as time passes.

Can this concept be quantified? In other words, can one say how much the disorder of the gas has increased after it has spread out to fill both chambers? Consider a single molecule in the gas. A molecule that can roam throughout both chambers has twice as many possible positions as a molecule confined to a single chamber: there are twice as many ways for a molecule to occupy the two-chamber apparatus. If there are two molecules in the two-chamber apparatus, each molecule has twice as many possible positions as it would have in a single chamber, and so the system as a whole has 2×2, or four, times as many possible configurations. If there are three molecules, the system has $2 \times 2 \times 2$, or eight, times as many possible configurations.

In general, if there are n molecules in the gas, the gas can fill two chambers in 2^n times more ways than it can fill a single chamber. The gas in the two-chamber apparatus is said to have 2^n times as many "accessible states" as the gas in a single chamber. In the same way, the number of accessible states in most systems depends exponentially on the number of molecules.

The entropy of a system is therefore defined as the logarithm of the number of accessible states. In the example of the two-chamber gas apparatus, a 2^n-fold increase in the number of accessible states is an increase in entropy of n bits, or binary units. (The base of the logarithm—and hence the size of a unit of entropy—is arbitrary; it is conventional to choose base 2 and binary units.) The logarithmic scale has the advantage of making the entropy of a sample of matter, like its energy or mass, roughly proportional to the number of molecules in the sample. One can draw an analogy to a computer memory: an n-bit memory, other things being equal, has size, weight and cost that are roughly proportional to n, although the number of distinct states possible in the memory is 2^n.

The earliest statements of the second law did not mention randomness or disorder; they concerned heat, work and temperature. How can these concepts be related to our quantitative definition of entropy?

The molecules in any sample of matter are always in motion. The speed and direction of each molecule are random, but the average speed of the molecules is proportional to the square root of the sample's temperature (as measured from absolute

zero). As the temperature of a sample is raised (and the average speed increases) the velocities of individual molecules come to be distributed over a greater range than they are when the average speed is low.

When the average speed is high, then, every molecule in the sample has a greater range of velocities available to it, just as a molecule in a two-chamber gas apparatus has a greater range of positions available to it than a molecule in a single-chamber apparatus has. There are thus more accessible states at high temperatures than there are at low temperatures. The motion is more disordered at high temperatures, because it is harder to predict what the velocity of any molecule will be.

Disorder of molecular motion and disorder of molecular positions must both be counted in determining the entropy of a system. The entropy of a gas can be increased either by allowing the gas to occupy a greater volume or by increasing its temperature so that its molecular motion becomes more disorderly.

Any flow of heat therefore carries entropy with it. To be precise, it turns out that a heat flow carries an amount of entropy proportional to the quantity of heat flowing divided by the temperature at which the flow takes place. Hence a flow from a hot body to a cold body raises the entropy of the cold body more than it lowers the entropy of the hot one: the same amount of heat leaves the hot body as enters the cold body, but in figuring the entropy decrease of the hot body one divides by a high temperature, whereas in figuring the entropy increase of the cold body one divides by a low temperature. A heat flow from a hot to a cold body thus raises the entropy of the universe.

Our more precise definition of entropy gives us a better understanding of why Maxwell's demon seems to violate the second law. By its sorting action the demon is causing heat to flow from room A to room B, even after room B has become warmer than room A. The demon is therefore lowering the entropy of room A by a greater amount than it is raising the entropy of room B. The demon therefore decreases the entropy of the universe as a whole—a thermodynamic impossibility.

In his description of the demon Maxwell made it clear he believed in the validity of the second law. He suggested that perhaps human beings are unable to violate the second law (by doing what the demon can do) simply because they lack the demon's ability to see and handle individual molecules. This is not a completely satisfying exorcism of the demon, because it leaves open the question of whether a being able to see and handle individual molecules, if such a being did exist, could violate the second law.

One way to uncover the reasons Maxwell's demon cannot work is to analyze and refute various simple, inanimate devices that might function as demons, such as the miniature spring-loaded trapdoor mentioned above, which acts as a one-way valve for molecules.

Imagine that the door opens to the left. If the demon works as it is supposed to, then every time a molecule from the room on the right strikes the door, the door swings open and the molecule passes into the room on the left. When a molecule from the left strikes the door, however, the door slams shut, trapping the molecule. Eventually all the molecules are trapped on the left, and the demon has compressed the gas (reducing its entropy) without doing any work.

How is the trapdoor demon flawed? First of all, the spring holding the door shut must be rather weak. The work of opening the door against the spring's force must be comparable to the average kinetic energy of the gas molecules. In 1912 Marian Smoluchowski pointed out that because the door is repeatedly being struck by molecules, it will eventually acquire its own kinetic energy of random motion (that is, heat energy). The door's energy of random motion will be about the same as that of the molecules striking it, and so the door will jiggle on its hinges and swing open and shut (remember that the door is very small), alternately bouncing against its jamb and swinging open against the force of the spring.

When the door is open, it obviously cannot function as a one-way valve, since molecules can pass freely in both directions. One might still hope that the door would act as an inefficient demon, trapping at least a small excess of gas on the left, but it cannot do even that. Any tendency the door has to act as a one-way valve, opening to let a molecule go from the right to the left, is exactly counteracted by its tendency to do the reverse: to slam shut against a molecule that has wandered in front of it, actively pushing the molecule from the room on the left to the one on the right (aided by the force of the spring).

The two processes—a molecule pushing its way past the door from right to left, and the door pushing a molecule from left to right—are me-
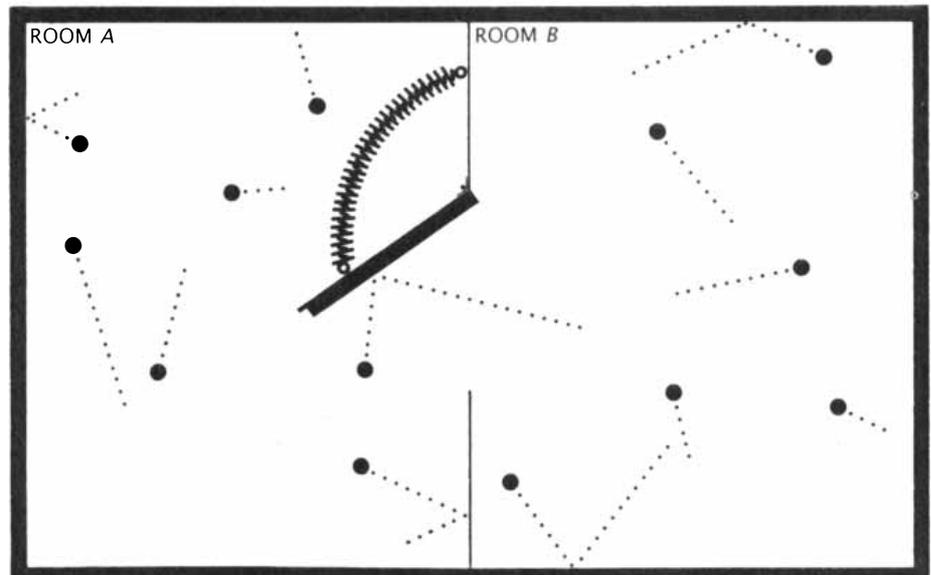
TRAPDOOR "DEMON" is a form of Maxwell's demon designed to operate automatically and to create an inequality of pressure, not of temperature. A spring-loaded trapdoor blocks a hole between two rooms initially containing gas at equal temperatures and pressures. The door swings open in only one direction in order to admit molecules from room B into room A but not vice versa. Eventually, one might think, molecules will accumulate in A at the expense of B, creating an inequality of pressure. Actually the inequality does not build up. The trapdoor, heated by collisions with molecules, jiggles open and closed randomly because of thermal energy. When it is open, it is not a one-way valve, and as it closes it may push a molecule from A into B. The latter process takes place as often as its inverse, in which a molecule from B pushes past the door into A.
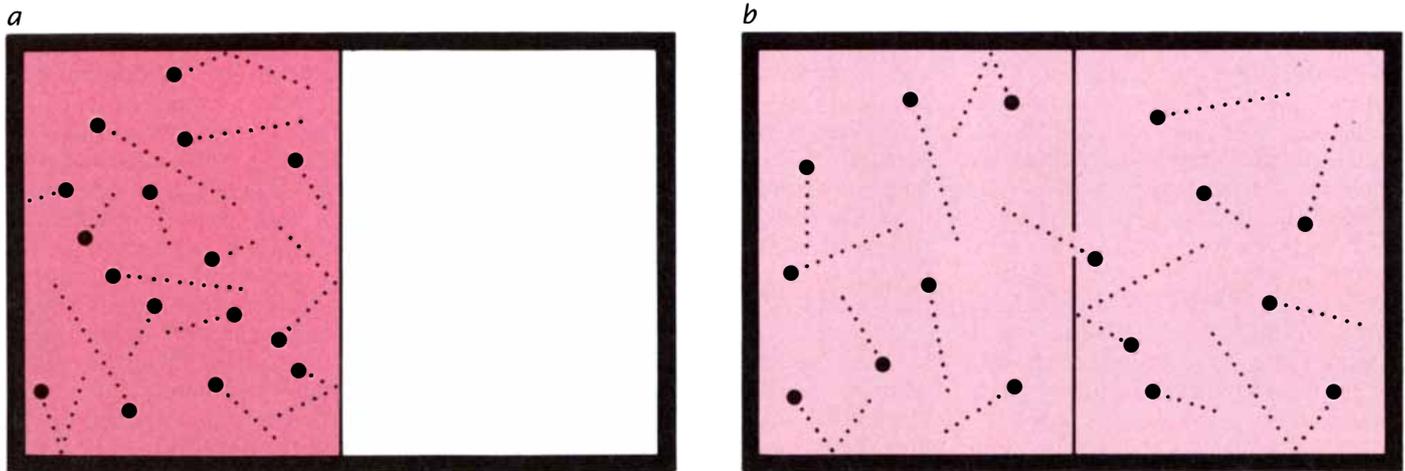
FREE EXPANSION of a gas is a thermodynamically irreversible process: one in which the entropy, or disorder, of the universe increases. A gas is initially confined in one chamber of a two- chamber apparatus (*a*). The barrier between the chambers is pierced, and molecules leak from one chamber into the other until approximately the same number of molecules are in both (*b*).

chanical reverses of each other: a motion picture of one, shown backward, would look like the other. In an environment at a constant temperature and pressure both processes would take place equally often, and the ability of the trapdoor to act as a one-way valve would be exactly zero. It cannot work as a demon.

In environments where the pressure is not equal on both sides of the door, of course, such devices do function. Large-scale versions, built with macroscopic doors and springs, can be seen on ventilator fans designed to blow stale air out of restaurants without admitting gusts of outside air when the fan is off. Microscopic versions would function in much the same way, allowing molecules to pass if there were excess pressure on one side but shutting off the flow if there were excess pressure on the other. The devices would not violate the second law, because they could only allow pressures to equalize; they could never form regions of excess pressure.

Even though a simple mechanical demon cannot work, perhaps an intelligent one can. Indeed, some time after Maxwell had described the demon, many investigators came to believe intelligence was the critical property that enabled the demon to operate. For example, in a 1914 paper Smoluchowski wrote: "As far as we know today, there is no automatic permanently effective perpetual-motion machine, in spite of the molecular fluctuations, but such a device might, perhaps, function regularly if it were appropriately operated by intelligent beings."

The physicist Leo Szilard attempted a quantitative analysis of this question in a paper published in 1929, "On the Decrease of Entropy in a Thermodynamic System by the Intervention of Intelligent Beings." Although the title seems to imply an intelligent demon could violate the second law, the body of the article is devoted to refuting this notion and to arguing that no being, intelligent or not, can do so. Szilard thought the observation, or measurement, the demon must make (for example, to see which side a molecule is coming from) cannot be done without also doing enough work to cause an increase in entropy sufficient to prevent a violation of the second law.

Szilard considered a demon that differed in several ways from Maxwell's; his demon has since come to be called Szilard's engine. (The engine I shall describe here differs slightly from Szilard's original one.) The engine's main component is a cylinder in which there is a single molecule in random thermal motion. Each end of the cylinder is blocked by a piston, and a thin, movable partition can be inserted in the middle of the cylinder to trap the molecule in one half of the cylinder or the other [*see illustration on opposite page*]. The engine is also equipped with devices for finding which half of the apparatus the molecule is in and a memory for recording that information.

The engine's cycle consists of six steps. In the first step the partition is inserted, trapping the molecule on one side or the other. Szilard argued that the work necessary to insert the partition can in principle be made negligibly small.

In the next step the engine determines which half of the apparatus the molecule has been trapped in. The engine's memory device has three possible states: a blank state to signify that no measurement has been made, an *L* to signify that the molecule has been observed in the left half of the apparatus, and an *R* to signify that the molecule has been observed in the right half. When the measurement is made, the memory switches from the blank state to one of the other two.

The third step, which might be called a compression stroke, depends on the knowledge gained during the preceding step. The piston on the side that does not contain the molecule is pushed in until it touches the partition. Unlike the compression stroke of an internal-combustion engine, this compression stroke requires no work, because the piston is "compressing" empty space; the molecule, which is trapped on the other side of the partition, cannot resist the piston's movement.

Then, in the fourth step, the partition is removed, allowing the molecule to collide with the piston that has just been advanced. The molecule's collisions exert a pressure on the face of the piston.

In the fifth step, which might be called the power stroke, the pressure of the molecule drives the piston backward to its original position, doing work on it. The energy the molecule gives to the piston is replaced by heat conducted through the cylinder walls from the environment, and so the molecule continues moving at the same average speed. The effect of the power stroke is therefore to convert heat from the surroundings into mechanical work done on the piston.

In the sixth step the engine erases its memory, returning it to the blank state. The engine now has exactly the same configuration it had at the

beginning of the cycle, and the cycle can be repeated.

Overall, the six steps appear to have converted heat from the surroundings into work while returning the gas and the engine to the same state they were in at the start. If no other change has occurred during the cycle of operation, the entropy of the universe as a whole has been lowered. In principle the cycle can be repeated as often as the experimenter wants, leading to an arbitrarily large violation of the second law.

Szilard's way out of this predicament was to postulate that the act of measurement, in which the molecule's position is determined, brings about an increase in entropy sufficient to compensate for the decrease in entropy brought about during the power stroke. Szilard was somewhat vague about the nature and location of the increase in entropy, but in the years after he published his paper a number of physicists, notably Leon Brillouin (the author, in 1956, of the widely read book *Science and Information Theory*) and Denis Gabor (best known as the inventor of holography), tried to substantiate the postulated irreversibility of measurement. In particular they tried to determine what the cost should be, in terms of energy and entropy, of observing a molecule by aiming light at it and observing the reflections.

In their work, Brillouin and Gabor drew on a theory that had been developed since Maxwell's time: the quantum theory of radiation. According to the classical wave theory of light (to which Maxwell made fundamental contributions), the energy of a light ray can be made arbitrarily small. According to the quantum theory, however, light consists of energy packets called photons. The energy of a photon depends on its wavelength, or color, and it is impossible to detect less than one photon of light. Brillouin argued that for a mole-

cule to be observed it must scatter at least one photon of a probe beam, and that when the photon's energy is dissipated into heat, the dissipation must produce an entropy increase at least as great as the entropy decrease Szilard's engine could achieve as the result of information gained about the scattering molecule.

Why not simply use a probe beam of photons that have very low energies? The scheme will not work, because of another, more complicated, consequence of the quantum theory. According to the quantum theory of radiation, any vessel whose walls and interior are all at a single constant temperature becomes filled with a "gas" of photons: a bath of radiation. The wavelengths of the photons depend on the temperature of the vessel. Such a photon gas constitutes the uniform red or orange glow inside a hot furnace. (At room temperature the photons are mostly in the infrared part of the spectrum and are therefore invisible.)

The photon gas might seem at first to be a handy source of light by which the demon could observe gas molecules (thereby saving itself the entropy cost of a flashlight). One of the surprising consequences of the second law, however (a consequence discovered by Gustav Robert Kirchhoff in 1859), is that it is impossible to see anything in a vessel at uniform temperature by the light of the vessel's own glow. If one looks into a kiln in which pots are being fired, for example, one will see a uniform orange glow almost devoid of contrast, even though the pots in the kiln may have very different colors, brightnesses and surface textures.

The objects in the hot kiln look as if they are all the same color and brightness, but they are not, as one can verify by shining a bright light on them from outside the kiln. The reason the objects nearly disappear by the light of the kiln must therefore

SZILARD ENGINE, modeled after a machine described in 1929 by Leo Szilard, seems to convert heat from its surroundings into work, contrary to the second law. The engine (*1*) is a cylinder that is blocked off at both ends by pistons; it is equipped with a movable partition and devices for observing the cylinder's contents and recording the results of observations. The cylinder contains a single molecule. At the start of the engine's cycle (*2*) the partition is lowered, trapping the molecule in one half of the cylinder. The observational devices determine and record which half contains the molecule (*3*), and the piston from the other half is pushed in until it touches the partition (*4*). Moving the piston requires no work, since it compresses empty space. Then the partition is withdrawn (*5*) and the molecule strikes the piston, pushing it backward (*6*). (The one-molecule gas "expands" against the piston.) Energy lost by the molecule as it works against the piston is replaced by heat from the environment. When the piston has returned to its original position (*7*), the memory is erased (*8*) and the cycle can begin again.

1

FRAME

KEEL

KEY

R   L

LOCKING PIN

2

R   L

3

R   L

4

R   L

5

R   L
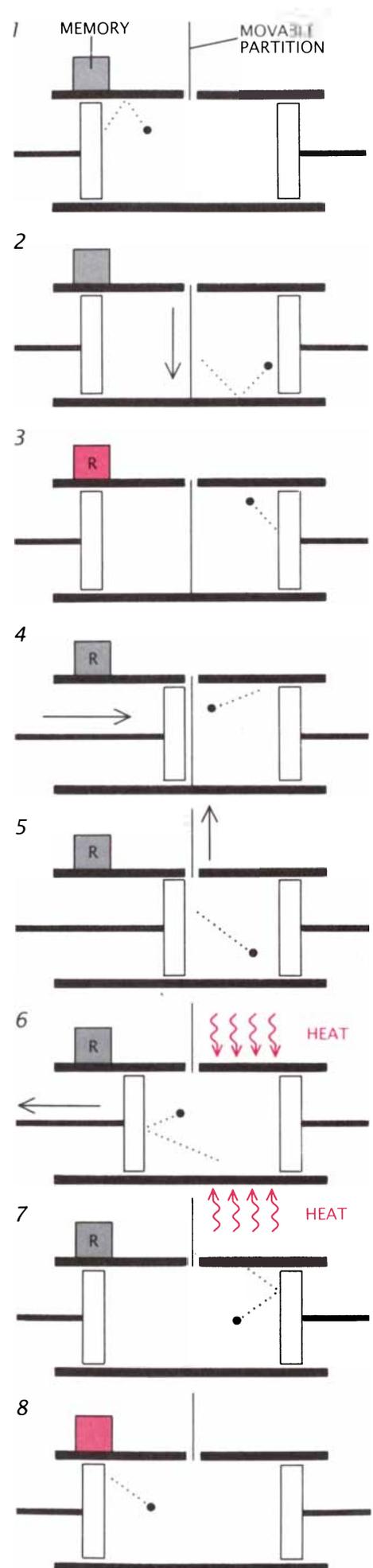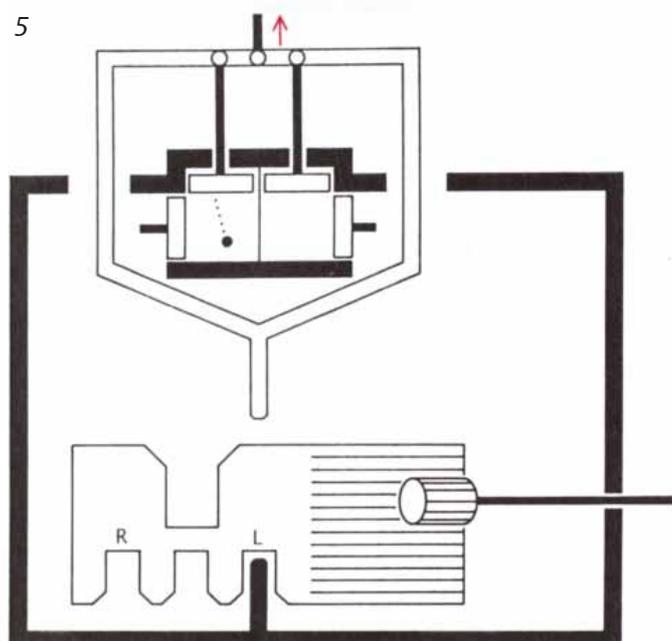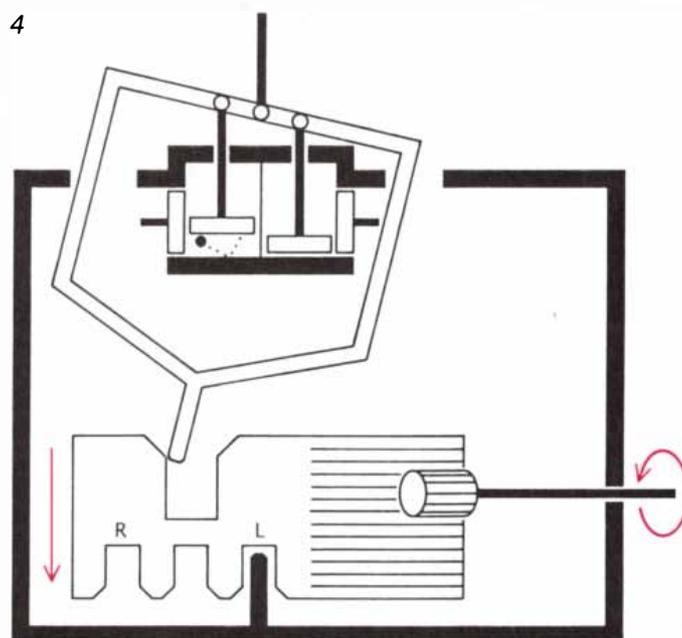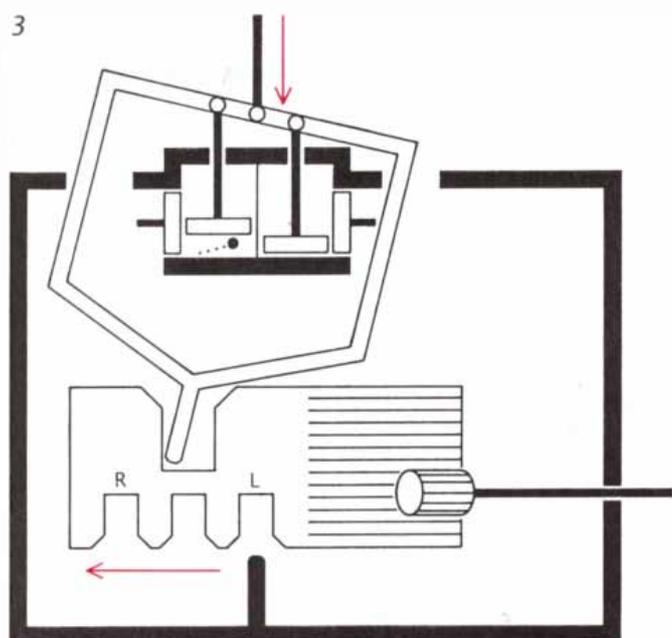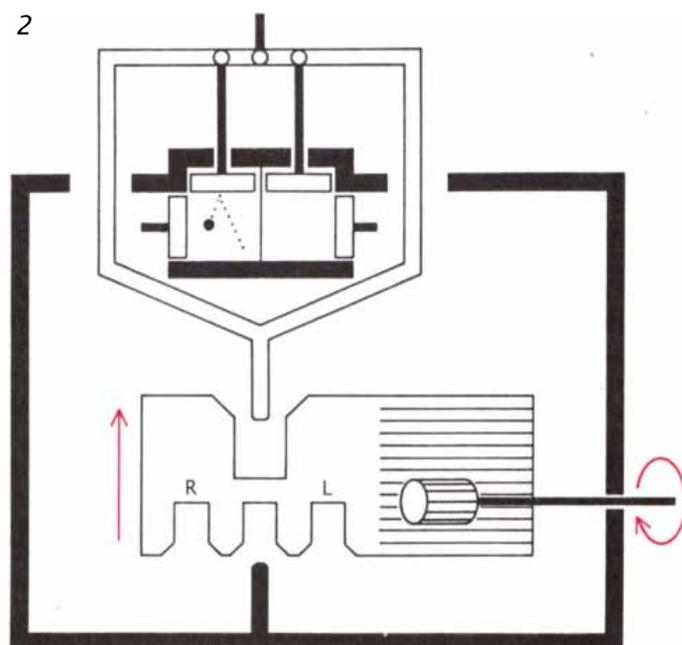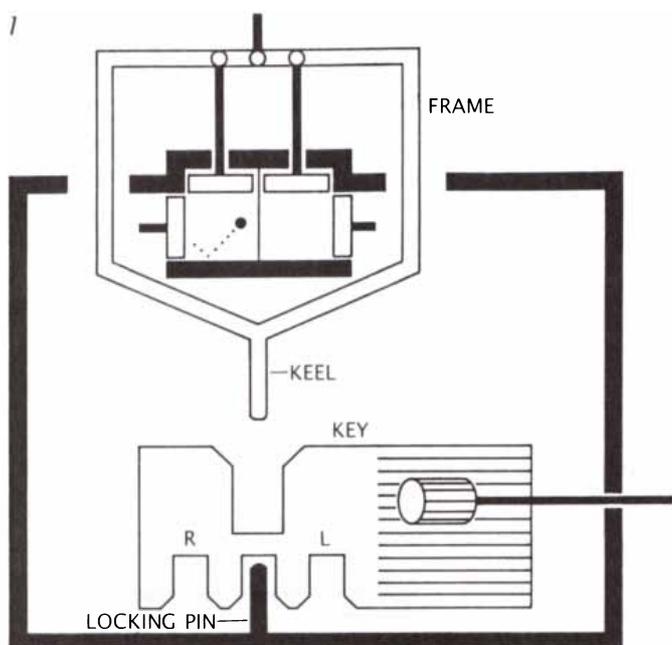
MEASUREMENT APPARATUS, designed by the author to fit the Szilard engine, determines which half of the cylinder the molecule is trapped in without doing appreciable work. A slightly modified Szilard engine sits near the top of the apparatus (*1*) within a boat-shaped frame; a second pair of pistons has replaced part of the cylinder wall. Below the frame is a key, whose position on a locking pin indicates the state of the machine's memory. At the start of the measurement the memory is in a neutral state, and the partition has been lowered so that the molecule is trapped in one side of the apparatus. To begin the measurement (*2*) the key is moved up so that it disengages from the locking pin and engages a "keel" at the bottom of the frame. Then the frame is pressed down (*3*). The piston in the half of the cylinder containing no molecule is able to descend completely, but the piston in the other half cannot, because of the pressure of the molecule. As a result the frame tilts and the keel pushes the key to one side. The key, in its new position, is moved down to engage the locking pin (*4*), and the frame is allowed to move back up (*5*), undoing any work that was done in compressing the molecule when the frame was pressed down. The key's position indicates which half of the cylinder the molecule is in, but the work required for the operation can be made negligible. To reverse the operation one would do the steps in reverse order.

be that dark (that is, nonreflective) objects glow proportionately more brightly than light (reflective) objects, so that the total light intensity leaving any object (reflected and emitted light combined) is the same.

To see why this strange leveling of intensity must take place, suppose it did not occur and think about the consequences for the second law. Suppose two objects, say a vase and a pot, are placed close together in a kiln at uniform temperature. If the intensity of light leaving the vase toward the pot were greater than that leaving the pot toward the vase, energy would flow from the vase to the pot. The pot would become warmer and the vase would become cooler.

Thus, without the expenditure of work, two regions that were once at a uniform temperature would come to different temperatures, just as if a Maxwell's demon had been sitting between them, and the second law would be violated. Therefore if the second law is to be valid, objects in a vessel at uniform temperature cannot have different surface intensities.

In order to see the objects in a furnace, then, one must shine light in from an external source, such as a flashlight that has a filament hotter than the furnace's temperature. In daily life such light sources—the sun, for example—make it possible for us to see objects in vessels that are uniformly at room temperature.

Brillouin, Gabor and others, armed with an understanding of the photon gas, argued that Maxwell's demon cannot observe the molecules it sorts without some kind of light source. Therefore, they said, the demon cannot violate the second law. Every time it observes a molecule the demon must dissipate the energy of at least one photon; the energy of that photon must be greater than a minimum energy determined by the temperature of the gas in which the demon sits. Such arguments, although they are not completely rigorous, seemed to substantiate Szilard's belief that acquiring a given amount of information entails producing a corresponding amount of entropy.

The next major progress toward banishing the demon was a side effect of research by Rolf Landauer of IBM on the thermodynamics of data processing. Certain data-processing operations, such as the copying of data from one device into another, are analogous to measurements, in that one device acquires information about the state of the other. Hence it

was generally believed in the 1950's that data-processing operations were intrinsically irreversible (in the thermodynamic sense of the word), just as Szilard had argued that measurement in general is irreversible. It was thought that any kind of data operation required the generation and removal of at least one bit's worth of heat for every bit of data to be processed. (This is an extremely small quantity of heat: roughly one ten-billionth of the heat actually generated by existing electronic circuits.)

In about 1960 Landauer analyzed the question more thoroughly. He found that some data operations are indeed thermodynamically costly but others, including, under certain conditions, copying data from one device to another, are free of any fundamental thermodynamic limit [see "The Fundamental Physical Limits of Computation," by Charles H. Bennett and Rolf Landauer; SCIENTIFIC AMERICAN, July, 1985].

Landauer's proof begins with the premise that distinct logical states of a computer must be represented by distinct physical states of the computer's hardware. For example, every possible state of the computer's memory must be represented by a distinct physical configuration (that is, a distinct set of currents, voltages, fields and so forth).

Suppose a memory register of n bits is cleared; in other words, suppose the value in each location is set at zero, regardless of the previous value. Before the operation the register as a whole could have been in any of 2^n states. After the operation the register can be in only one state. The operation has therefore compressed many logical states into one, much as a piston might compress a gas.

By Landauer's premise, in order to compress a computer's logical state one must also compress its physical state: one must lower the entropy of its hardware. According to the second law, this decrease in the entropy of the computer's hardware cannot be accomplished without a compensating increase in the entropy of the computer's environment. Hence one cannot clear a memory register without generating heat and adding to the entropy of the environment. Clearing a memory is a thermodynamically irreversible operation.

Landauer identified several other operations that are thermodynamically irreversible. What all these operations have in common is that they discard information about the computer's past state. In Landauer's

phrase, such operations are "logically irreversible."

The connection of these ideas to the problem of the measurement, implicit in Landauer's work and in the reversible models of computation developed during the 1970's by Edward Fredkin of M.I.T., myself and others, became explicit in 1982, when I proposed that they provide the correct explanation of Maxwell's demon. Consider the operating cycle of Szilard's engine. The last step, in which the engine's memory is reset to a blank state, is logically irreversible, because it compresses two states of the machine's memory ("The molecule is on the left" and "The molecule is on the right") into one ("The molecule's position has not yet been measured"). Thus the engine cannot reset its memory without adding at least one bit of entropy to the environment. This converts all the work that had been gained in the power stroke back into heat.

What about the measurement step? Is it thermodynamically costly as well? In that case the engine would add to the entropy of the universe twice: once in measuring the molecule's position and again in resetting its memory after the power stroke. Actually the measurement does not have to be thermodynamically costly. There are ways to observe molecules other than by bouncing light off them. To prove this point I have designed a reversible measuring device, which measures and records the position of the molecule without undergoing any thermodynamically irreversible steps.

We have, then, found the reason the demon cannot violate the second law: in order to observe a molecule, it must first forget the results of previous observations. Forgetting results, or discarding information, is thermodynamically costly.

If the demon had a very large memory, of course, it could simply remember the results of all its measurements. There would then be no logically irreversible step and the engine would convert one bit's worth of heat into work in each cycle. The trouble is that the cycle would not then be a true cycle: every time around, the engine's memory, initially blank, would acquire another random bit. The correct thermodynamic interpretation of this situation would be to say the engine increases the entropy of its memory in order to decrease the entropy of its environment.

Attributing the gain in entropy to

the resetting step rather than to the measurement step may seem to be a mere bookkeeping formality, since any complete cycle of Szilard's engine must include both steps, but considerable confusion can be avoided if one draws a clear distinction between the acquisition of new information and the destruction of old information. The confusion may or may not have existed in Szilard's mind. In most of his paper he refers to measurement as the irreversible step, but at one point he makes an accounting of entropy changes during the cycle and finds, without explicitly commenting on it, that the increase in entropy takes place during the resetting of the memory.

If subsequent workers had pursued this aspect of Szilard's paper, they would have come to our present understanding of Maxwell's demon. Their failure to do so is an irony in the history of science: the advancement of one branch of physics (the quantum theory of radiation) apparently delayed progress in another branch (thermodynamics). One aspect of quantum mechanics that reinforced the idea that a fundamental thermodynamic price must be paid for acquiring information is the uncertainty principle, which holds that certain sets of measurements cannot be carried out with more than a certain degree of precision. Although the uncertainty principle sounds similar to Szilard's hypothesis that measurements have an irreducible entropy cost, in fact it is fundamentally different. Szilard's hypothesis concerns the thermodynamic cost of measurements, whereas the uncertainty principle concerns the possibility of their being made at all, whatever their thermodynamic cost.

Another source of confusion is that we do not generally think of information as a liability. We pay to have newspapers delivered, not taken away. Intuitively, the demon's record of past actions seems to be a valuable (or at worst a useless) commodity. But for the demon "yesterday's newspaper" (the result of a previous measurement) takes up valuable space, and the cost of clearing that space neutralizes the benefit the demon derived from the newspaper when it was fresh. Perhaps the increasing awareness of environmental pollution and the information explosion brought on by computers have made the idea that information can have a negative value seem more natural now than it would have seemed earlier in this century.

The role of quantum information in thermodynamics—a topical review

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Topical Review

The role of quantum information in thermodynamics—a topical review

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Abstract

This topical review article gives an overview of the interplay between quantum information theory and thermodynamics of quantum systems. We focus on several trending topics including the foundations of statistical mechanics, resource theories, entanglement in thermodynamic settings, fluctuation theorems and thermal machines. This is not a comprehensive review of the diverse field of quantum thermodynamics; rather, it is a convenient entry point for the thermo-curious information theorist. Furthermore this review should facilitate the unification and understanding of different interdisciplinary approaches emerging in research groups around the world.

Keywords: quantum information, thermodynamics, resource theories, thermalization, entanglement, fluctuations

(Some figures may appear in colour only in the online journal)

1. Introduction

If physical theories were people, thermodynamics would be the village witch. Over the course of three centuries, she smiled quietly as other theories rose and withered, surviving major revolutions in physics, like the advent of general relativity and quantum mechanics. The other theories find her somewhat odd, somehow *different* in nature from the rest, yet everyone comes to her for advice, and no-one dares to contradict her. Einstein, for instance, called her

'the only physical theory of universal content, which I am convinced, that within the framework of applicability of its basic concepts will never be overthrown.'

Her power and resilience lay mostly on her frank intentions: thermodynamics has never claimed to be a means to understand the mysteries of the natural world, but rather a path towards efficient exploitation of said world. She tells us how to make the most of some resources, like a hot gas or a magnetized metal, to achieve specific goals, be them moving a train or formatting a hard drive. Her universality comes from the fact that she does not try to understand the microscopic details of particular systems. Instead, she only cares to identify which operations are easy and hard to implement in those systems, and which resources are freely available to an experimenter, in order to quantify the cost of state transformations. Although it may stand out within physics, this operational approach can be found in branches of computer science, economics and mathematics, and it plays a central role in quantum information theory—which is arguably why quantum information, a toddler among physical theories, is bringing so much to thermodynamics.

In the early twentieth century, information theory was constructed as the epitome of detachment from physics [7]. Its basic premise was that we could think of information independently of its physical support: a message in a bottle, a bit string and a sensitive phone call could all be treated in the same way. This level of abstraction was not originally conceived for its elegance; rather, it emerged as the natural way to address very earthly questions, such as 'can I reliably send a message through a noisy line?' and 'how much space do I need to store a picture?'. In trying to quantify the resources required by those tasks (for example, the number of uses of the noisy channel, or of memory bits), it soon became clear that the relevant quantities were variations of what is now generally known as entropy [8]. *Entropy measures* quantify our uncertainty about events: they can tell us how likely we are to guess the outcome of a coin toss, or the content of a message, given some side knowledge we might have. As such, they depend only on probability distributions over those events, and not on their actual content (when computing the odds, is does not matter whether they apply to a coin toss or to a horse race). Information theory has been greatly successful in this approach, and is used in fields from file compression to practical cryptography and channel coding [8].

But as it turned out, not all information was created equal. If we zoom in and try to encode information in the tiniest support possible, say the spin of an electron, we face some of the perplexing aspects of quantum physics: we can write in any real number, but it is only possible to read one bit out, we cannot copy information, and we find correlations that cannot be explained by local theories. In short, we could not simply apply the old information theory to tasks involving quantum particles, and the scattered study of quirky quantum effects soon evolved into the fully-fledged discipline of quantum information theory [9]. Today we see quantum theory as a generalization of classical probability theory, with density matrices replacing probability distributions, measurements taking the place of events, and quantum entropy measures to characterize operational tasks [10].

While quantum information theory has helped us understand the nature of the quantum world, its practical applications are not as well spread as for its classical counterpart. Technology is simply not there yet—not at the point where we may craft, transport and preserve all the quantum states necessary in a large scale. These technical limitations, together with a desire to pin down exactly what makes quantum special, gave rise to resource theories within quantum information, for instance theories of entanglement [13]. There, the rough premise is that entangled states are useful for many interesting tasks (like secret key sharing), but distributing entanglement over two or more agents by transporting quantum particles over a distance is hard, as there are always losses in the process [14]. Therefore, all entangled states become a precious resource, and we study how to distill entanglement from them using only a

set of allowed operations, which are deemed to be easier to implement—most notoriously, local operations and classical communication (LOCC) [15].

Other resource theories started to emerge within quantum information—purity and asymmetry have also been framed as resources under different sets of constraints—and this way of thinking quickly spread among the quantum information community (see [16] for a review). As many of its members have a background in physics and an appetite for abstraction, it was a natural step for them to approach thermodynamics with such a framework in mind. Their results strengthen thermodynamics, not only by extending her range of applicability to small quantum systems, but also by revisiting her fundamental principles. The resource theory approach to thermodynamics is reviewed in section 4.

Each resource theory explores the limitations imposed by one specific physical constraint, like locality or energy conservation. In a realistic setting we could be bound to several of these constraints, a natural case that can be modelled by combining different resource theories, thus restricting the set of allowed operations. In section 5 we review and discuss attempts to combine thermodynamic and locality constraints. In particular, we look at the role of entanglement resources in thermodynamic tasks, thermodynamic witnesses of non-classicality, and entanglement witnesses in phase transitions.

Information theory also shed light on fundamental issues in statistical mechanics—the mathematical backbone of thermodynamics. Perhaps one of the earliest significant contributions is the maximal entropy principle introduced by Jaynes [17, 18]. In these seminal works Jaynes addresses the issue of justifying the methods of statistical mechanics from microscopic mechanical laws (classical or quantum) using tools from information theory. In fact, deriving statistical mechanics, and hence thermodynamics from quantum mechanics is almost as old as quantum mechanics itself starting with the work of von Neumann [11, 19]. This is very much an ongoing and active research area and in recent years has received significant attention from the quantum information community. The most significant contributions are reviewed in section 3.

In the past twenty years, the field of non-equilibrium statistical mechanics has seen a rapid development in the treatment of driven classical and quantum systems beyond the linear response regime. This has culminated in the discovery of various fluctuation theorems which relate equilibrium thermodynamic quantities to non-equilibrium ones, and led to a revision on how we understand the thermodynamics of systems far from equilibrium [20–24]. Although this approach is relatively recent from a statistical physics perspective, a cross-fertilization with concepts ubiquitous in quantum information theory has already started, including phase estimation techniques for extraction of work and heat statistics and feedback fluctuation theorems for Maxwell's demons. In section 6 we identify these existing relationships and review areas where more overlap could be developed.

As ideas and concepts emerge and develop it is not surprising that quantum information theorists have started to turn towards the pragmatic goal of describing the advantages and disadvantages of machines which operate at and below the quantum threshold. Although ideas relating quantum engines have been around for a long time [25–27]—questions pertaining to the intrinsic quantumness in the functioning of such machines have been raised using the tools of quantum information theory only relatively recently. We review progress along these lines in section 7.

1.1. Scope and other reviews

This review focuses on landmark and recent articles in the field of quantum thermodynamics with a special emphasis on contributions from quantum information theory. We place emphasis on current trending topics, discuss different approaches and models and peek into

the future directions of the field. As the review is 'topical', we focus on the interplay between quantum information and thermodynamics. Readers from different communities will get an overview of how concepts and techniques from their fields have been applied to thermodynamics.

As the vastness of possible topics could easily exceed the scope of a topical review, we refer to other review articles and books concerning questions that have already been covered by other authors:

- *Equilibration and thermalization.* Recovering statistical mechanics from the unitary evolution of a closed quantum system is an issue which is almost as old as quantum mechanics itself. This topic, far from being an academic issue, has seen an unprecedented revival of interest due mainly to advances in experimental ultra-cold atoms. We discus the topic in section 3, from a quantum information perspective. This topic is more extensively reviewed in [28]. For readers interested in this topic from a condensed matter perspective we recommend the review [29] and the special issue [30] for more recent developments.
- *Thermal machines.* As mentioned in the introduction viewing engine cycles from a fully quantum mechanical perspective is also not a new topic [25–27]. Many results on quantum engines exist which are not directly related to quantum information processing we exclude them from section 7 and the interested reader may learn more in [31–33].
- *Maxwell's demon and Landauer's principle.* Almost as old as thermodynamics itself is the Maxwell's demon paradox, briefly introduced in figure 1 and example 3. The demon paradox inspired the seminal work of Szilard to reformulate the demon as a binary decision problem [34]. The resolution of Maxwell demon paradox by Landauer cements the relationship between the physical and information theoretical worlds. This demon has been extensively investigated from both a quantum and classical perspective in [2–6].
- *Quantum thermodynamics.* The 2009 book [35] covers a range of topics regarding the emergence of thermodynamic behaviour in composite quantum systems.
- *Entanglement and phase transitions in condensed matter.* Entanglement is frequently used as an indicator of quantum phase transitions in condensed matter systems. We do not cover this particular setting but the interested reader may find a comprehensive review in [36].
- *Resource theories.* Examples and common features of resource theories (beyond quantum information theory) are discussed in [37]. In particular, different approaches to general frameworks are discussed in section 10 of that work.
- *Experimental implementations.* Experiments with demons, thermal engines and work extraction are discussed in more depth in the   perspective article [38].

Definitions and notation.   Conventions followed unless otherwise stated:

States. Discrete Hilbert spaces $\mathbb{C}^d$. States ρ are represented by Hermitian matrices ($\mathrm{Tr}(\rho) = 1$ and $\rho \geqslant 0$). Subsystems are denoted by Roman subscripts, $\rho_\mathrm{A} := \mathrm{Tr}_\mathrm{B}(\rho_\mathrm{AB})$.

Entropy. Von Neumann entropy (see figure 2) with base 2 logarithm, $S(\rho) = -\mathrm{tr}(\rho \, \log_2(\rho))$.

Mutual information. Measures correlations, $I(A:B)_\rho := S(\rho_\mathrm{A}) + S(\rho_\mathrm{B}) - S(\rho_\mathrm{AB})$.

Energy. Hamiltonian H, average energy $\langle H \rangle_\rho = \mathrm{tr}(\rho H)$, eigenvalues $\{E_k\}_k$, eigenvectors $\{|E_k\rangle\}_k$, or $\{|E_k^i\rangle\}_{k,i}$ if there are degeneracies, with energy projectors $\Pi_k = \sum_i |E_k^i\rangle\langle E_k^i|$.

Thermal states. Gibbs state $\tau(\beta) = \frac{\mathrm{e}^{-\beta H}}{\mathcal{Z}}$, with partition function $\mathcal{Z} = \mathrm{Tr}(\mathrm{e}^{-\beta H})$ and inverse temperature $\beta := \frac{1}{k_\mathrm{B} T}$.

An early puzzle in thermodynamics: imagine a box filled with a gas, with a partition in the middle. An agent (the demon) who can observe the microscopic details of the gas particles, controls a small gate in the partition, selectively opening it to let slow particles flow to the left and fast ones to the right. This creates a temperature differential between the two sides. The demon can exploit this difference to extract work, by letting the hot gas on the right expand. This apparent contradiction with the second law of thermodynamics can be easily explained from an information-theoretical viewpoint. The demon had access to much more information than the standard observer assumed in the derivation of traditional thermodynamics, who can only read a few macroscopic parameters of a gas and assumes a uniform distribution over all compatible micro-states. Therefore, it seems natural that the demon may extract more work than predicted by standard thermodynamics—and this insight motivates the need for thinking of thermodynamics as a subjective resource theory, and extending it to the quantum regime. In the larger picture, Bennett showed that the amount of work needed to erase the demon's memory at the end of the procedure (or equivalently, to prepare the memory to store the necessary information on the particles in the beginning) precisely makes up for the work extracted [1]. For reviews, see [2-6].

Figure 1. Maxwell's demon.

Free energy. $F_\beta(\rho) := \langle H \rangle_\rho - \frac{1}{\ln(2)\beta} S(\rho)$.

Linbladian. $\mathcal{L}(\rho)$ generates Markovian, time-homogeneous, non-unitary dynamics.

2. Foundations of statistical mechanics

At first sight, thermodynamics and quantum theory are incompatible. While thermodynamics and statistical mechanics state that the entropy of the Universe as a whole is a monotonically increasing quantity, according to quantum theory the entropy of the Universe is constant since it evolves unitarily. This leads us to the question of to which extent the methods of statistical physics can be justified from the microscopic theory of quantum mechanics and both theories can be made compatible. Unlike classical mechanics, quantum mechanics has a way to circumvent this paradox: *entanglement*. We observe entropy to grow in physical systems

In 1932, von Neumann designed this thought experiment to determine the entropy of a density operator ρ [11]. The experiment accounts for the work cost of erasing the state of a gas of n atoms, initially in an ensemble $\rho^{\otimes n}$, with $\rho = \sum_k p_k |\phi_k\rangle \langle\phi_k|$, by transforming it into a pure state $|\phi_1\rangle^{\otimes n}$ by means of a *reversible* process.

It consists of 3 steps: 1. *Separation of the species*: the atoms in different states $|\phi_1\rangle,\ldots,|\phi_m\rangle$ inside a box of volume V are separated in different boxes of the same volume V by means of semi-permeable walls (from a to b and finally c). Note that no work has been done and no heat has been exchanged. 2. *Compression*: every gas $|\phi_k\rangle$ is isothermally compressed to a volume $V_k = p_k V$ (from c to d). The mechanical work done in that process is $W_k = n p_k \ln(V_k/V) = p_k \ln p_k$. The total entropy increase per particle of that process is $\Delta S = \sum_k p_k \ln p_k$. 3. *Unitary transformation*: every gas is put in the $|\phi_1\rangle$ state by applying different unitary transformations $|\phi_k\rangle \rightarrow |\phi_1\rangle$, which are taken for free (from d to e). As the entropy of the final state is zero, the entropy of the initial ensemble reads $S(\rho) = -\operatorname{Tr}(\rho \ln \rho)$.

Historically, it is remarkable that the Shannon entropy, which can be seen as a particular case of the von Neumann entropy for classical ensembles, was not introduced until 1948 [7], and Landauer's principle was proposed only in 1961 [12].

Figure 2. The thermodynamic origin of the von Neumann entropy.

because they are entangled with the rest of the Universe. In this section we review the progress made on this topic in recent years which show that equilibration and thermalization are intrinsic to quantum theory.

2.1. Equal a priori probabilities postulate as a consequence of typicality in Hilbert spaces

Let us consider a closed system that evolves in time restricted to some global constraint. The principle of *equal a priori probabilities* states that, at equilibrium, the system is equally likely to be found in any of its accessible states. This assumption lies at the heart of statistical mechanics since it allows for the computation of equilibrium expectation values by

performing averages on the phase space. However, there is no reason in the laws of mechanics (and quantum mechanics) to suggest that the system explores its set of accessible states uniformly. Therefore, the *equal a priori probabilities* principle has to be put in by hand.

One of the main insights from the field of quantum information theory to statistical mechanics is the substitution of the *Equal a priori probabilities postulate* by the use of *typicality* arguments [39, 40]. To be more precise, let us consider a quantum system described by a Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_B$ where $\mathcal{H}_S$ contains the degrees of freedom that are experimentally accessible and $\mathcal{H}_B$ the ones that are not. In practice, we think of S as a subsystem that we can access, and B as its environment (sometimes called the bath). Concerning the global constraint, in classical mechanics, it is defined by the constants of motion of the system. In quantum mechanics, we model the restriction as a subspace $\mathcal{H}_R \subseteq \mathcal{H}_S \otimes \mathcal{H}_B$. Let us denote by d_R, d_S and d_B the dimensions of the Hilbert spaces $\mathcal{H}_R$, $\mathcal{H}_S$ and $\mathcal{H}_B$ respectively.

The equal *a priori* probability principle would describe the equilibrium state as

$$\varepsilon_R = \frac{1_R}{d_R} \,, \tag{1}$$

and would imply the state of the subsystem S to be

$$\Omega_S = \mathrm{Tr}_B \varepsilon_R \,. \tag{2}$$

In [39] it is shown that, if we look only at the subsystem S, most of the states in $\mathcal{H}_R$ are indistinguishable from the equal *a priori* probability state, i.e. for most $|\psi\rangle \in \mathcal{H}_R$, $\mathrm{Tr}_B |\psi\rangle\langle\psi| \approx \Omega_S$. More explicitly, if $|\psi\rangle$ is randomly chosen in $\mathcal{H}_R$ according to the uniform distribution given by the Haar measure, then the probability that $\mathrm{Tr}_B |\psi\rangle\langle\psi|$ can be distinguished from Ω_S decreases exponentially with the dimension of $\mathcal{H}_R$, d_R

$$\mathrm{Prob}[\| \mathrm{Tr}_B(|\psi\rangle\langle\psi|) - \Omega_S \|_1 \geqslant d_R^{-1/3}] \leqslant 2\exp\left(-Cd_R^{1/3}\right), \tag{3}$$

where C is a constant and $\|\cdot\|_1$ is the trace norm. The trace norm $\|\rho - \sigma\|_1$ measures the physical distinguishability between the states ρ and σ in the sense that a $\|\rho - \sigma\|_1 = \sup_{O \leqslant 1}|\mathrm{Tr}(O\rho) - \mathrm{Tr}(O\sigma)|$, where the maximization is made over all the observables O with operator norm bounded by 1. The proof of equation (3) relies upon concentration of measure and in particular on *Levy's Lemma* (see [39] for details). Let us mention that ideas in this spirit can be already found in Lloyd's PhD Thesis [41] published in 1991. In particular, he presents bounds on how the expectation values of a fixed operator taken over random pure states of a restricted subspace fluctuate.

The weakness of the previous result lies in that the use of typicality is made in the whole subspace $\mathcal{H}_R$ and, as we will justify next, this is not a physical assumption. In nature, Hamiltonians have local interactions and systems evolve for times that are much smaller than the age of the Universe. Most states in the Hilbert space simply cannot be generated by evolving an initial product state under an arbitrary time-dependent local Hamiltonian in a time that scales polynomially in the system size [42]. Therefore, sampling uniformly from the whole Hilbert space is not physically meaningful. There has been a strong effort to generalize the concept of typicality for different sets of states [43–45].

The first 'realistic' set of states in which typicality was studied was the set of *matrix product states* (MPS) [46, 47]. These type of states have been proven to describe ground states of one-dimensional gapped Hamiltonians. They are characterized by the rank of a bipartition of the state. This parameter quantifies the maximum entanglement between partitions of an MPS. The MPSs with fixed rank form a set of states with an efficient classical representation (they only require polynomial resources in the number of particles). In [43], it

Scheme of the restricted subspace $\mathcal{H}_R$ with its untypical states forming little islands coloured in yellow. The left trajectory (dashed line) passes mostly on typical states while the right trajectory (solid line) has a non-negligible support on states that are not typical.
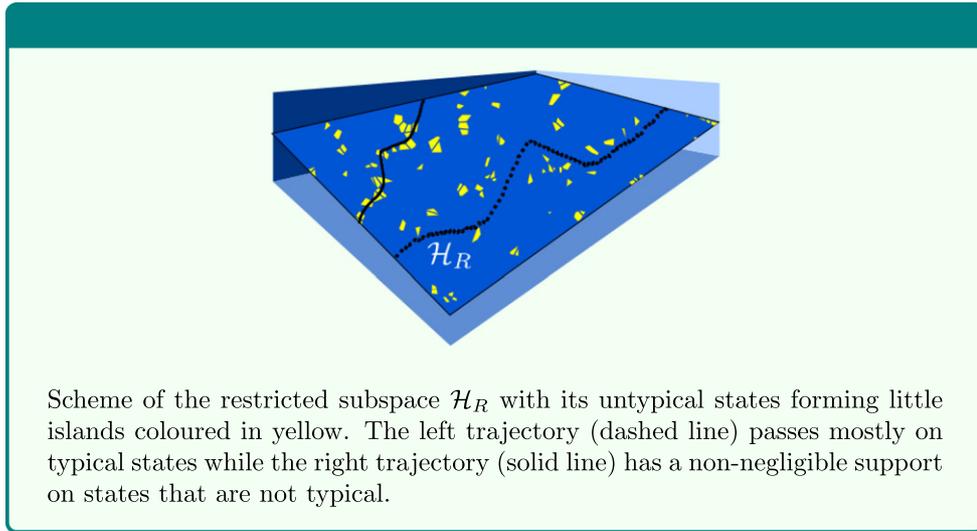
Figure 3. Typical and untypical trajectories.

is proven that typicality occurs for the expectation value of subsystems observables when the rank of the MPS scales polynomially with the size of the system with a power greater than 2.

Another set recently considered in the literature has been the so called set of *physical states* which consists of all states that can be produced by evolving an initial product state with a local Hamiltonian for a time polynomial in the number of particles *n*. By Trotter decomposing the Hamiltonian, such a set can be proven to be equivalent to the set of local *random quantum circuits*, that is, quantum circuits of qubits composed of polynomially many nearest neighbour two-qubit gates [42]. In [48], it was shown that the local random quantum circuits form an approximate unitary two-design, i.e. that random circuits of only polynomial length will approximate the first and second moments of the Haar distribution. In [44] the previous work was extended to poly(*n*)-designs. Finally, let us mention that the entanglement properties of typical *physical states* were studied in [45].

Let us mention that *k*-designs also appear naturally in the context of *decoupling theorems* in which a the subsystem *S* undergoes a physical evolution separated from the environment *B*, and one wonders under what conditions this evolution destroys all initial correlations between *S* and *B*. In particular, in [49] it is shown that almost-two-designs decouple the subsystem *S* from *B* independently of *B*'s size.

Another objection against typicality is that there are many physically interesting systems, e.g. integrable models, which, although their initial state belongs to a certain restricted subspace $\mathcal{H}_R$, their expectation values differ from the completely mixed state in *R*, ε_R, as expected from typicality arguments. This is a consequence of the fact that their trajectories in the Hilbert subspace $\mathcal{H}_R$ do not lie for the overwhelming majority of times on *generic* states (see figure 3). Hence, in practice, statements on equilibration and thermalization will depend on the dynamical properties of every system, that is, on their Hamiltonian. This leads us to the notion of *dynamical typicality*. In contrast to the *kinematic typicality* presented in this section, where an ensemble has been defined by all the states that belong to a certain subspace, in *dynamical typicality* the ensemble is defined by all states that share the same constants of motion given a Hamiltonian *H* and an initial state $|\psi(0)\rangle$. Studying whether typicality also holds in such a set will be precisely the problem addressed in the next section.

2.2. Equilibration. Maximum entropy principle from quantum dynamics

In this context of deriving thermodynamics from quantum mechanics the first problem that needs to be addressed is *equilibration*, that is, understand how the reversible unitary dynamics of quantum mechanics make systems equilibrate and evolve towards a certain state where they remain thereafter.

Because of the unitary dynamics, equilibration is only possible if the set of observables is restricted. In this spirit, a set of sufficient conditions for equilibration towards the time averaged state has been presented for local observables [50, 51] and observables of finite precision [52, 53]. The two approaches are proven to be equivalent in [54] and it is remarkable that the conditions given are weak and naturally fulfilled in realistic situations.

For simplicity, let us here focus on equilibration of subsystems and, as above, identify in the total system a subsystem S and its environment B. The dynamics of the total system are governed by the Hamiltonian H with eigenvalues $\{E_k\}_k$ and eigenvectors $\{|E_k\rangle\}_k$. This leads to the time evolution $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$ and the reduced state of S is $\rho_S(t) = \text{Tr}_B\rho(t)$ with $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$.

If equilibration happens, then it happens towards the time averaged state i.e. $\omega_S := \text{Tr}_B\omega$ with

$$\omega = \lim_{T\to\infty}\frac{1}{T}\int_0^T \rho(t)\,\mathrm{d}t = \sum_k P_k\rho(0)P_k \tag{4}$$

with P_k the projectors onto the Hamiltonian eigenspaces. The time averaged state is the initial state dephased in the Hamiltonian eigenbasis. For this reason it is also called *diagonal ensemble*.

In [50], a notion of equilibration is introduced by means of the average distance (in time) of the subsystem $\rho_S(t)$ from equilibrium. A subsystem S is said to equilibrate if

$$\langle\|\rho_S(t) - \omega_S\|_1\rangle_t := \lim_{T\to\infty}\frac{1}{T}\int_0^T \mathrm{d}t\,\|\rho_S(t) - \omega_S\|_1 \ll 1, \tag{5}$$

where $\|\rho_S(t) - \omega_S\|_1$ is the trace distance. If this average trace distance can be proven to be small, then the subsystem S is indistinguishable from being at equilibrium for almost all times.

Equilibration as a genuine property of quantum mechanics is shown in [50] by precisely proving that this average distance is typically small. More concretely, if the Hamiltonian that dictates the evolution of the system has *non-degenerate gaps* i.e. all the gaps of the Hamiltonian are different (an assumption which we will comment on below), then the average distance from equilibrium is bounded by

$$\langle\|\rho_S(t) - \omega_S\|_1\rangle_t \leqslant \sqrt{\frac{d_S}{d^{\text{eff}}(\omega^B)}} \leqslant \sqrt{\frac{d_S^2}{d^{\text{eff}}(\omega)}}, \tag{6}$$

where $d^{\text{eff}}(\rho) := 1/\text{Tr}(\rho^2)$ is the *effective dimension* of ρ and $\omega_B = \text{Tr}_S\omega$. Roughly speaking, the effective dimension of a state tells us how many eigenstates of the Hamiltonian support such state. It can also be related to the two-Renyi entanglement entropy by $S_2(\rho) = \log d^{\text{eff}}(\rho)$. Hence, equation (6) guarantees equilibration for Hamiltonians with non-degenerate energy gaps as long as the initial state is spread over many different energies.

Although the condition of having non-degenerate gaps may look very restrictive at first sight, note that Hamiltonians that do not fulfil it form a set of zero measure in the set of Hamiltonians, since any arbitrarily weak perturbation breaks the degeneracy of the gaps. In [51], the non-degenerate gaps condition was weakened by showing that equilibration occurs

provided that no energy gap is hugely degenerate. This condition can be understood as a way of preventing the situation where there is a subsystem which does not interact with the rest.

Let us finally point out that the equilibrium state introduced in equation (4) is precisely the state that maximizes the von Neumann entropy given all the conserved quantities [55]. This observation turns the *principle of maximum entropy* into a consequence of the quantum dynamics. The principle of maximum entropy was introduced by Jaynes in [17] and states that the probability distribution which best represents the current state of knowledge of the system is the one with largest entropy given the conserved quantities of the system. We will come back in more detail to the Jaynes principle in the next section when the thermalization for integrable systems is discussed.

2.3. Thermalization. Emergence of Gibbs states in local Hamiltonians

The next step in this program of justifying the methods of statistical mechanics from quantum mechanics is to tackle the issue of thermalization, i.e. to understand why the equilibrium state is usually well described by a Gibbs state, which is totally independent of the initial state of the system, except for some macroscopic constraints such as its mean energy. In [56], a set of sufficient conditions for the emergence of Gibbs states is presented for the case of a subsystem S that interacts weakly with its environment B through a coupling V. The Hamiltonian that describes such a situation is $H = H_S + H_B + V$. These conditions are a natural translation of the three ingredients that enter the standard textbook proof of the canonical ensemble in classical statistical physics:

 (i) The *equal a priory probability postulate* that has been replaced by typicality arguments in section 3.1, and an equilibration postulate (such as the second law) that has been replaced by quantum dynamics in section 3.2.
 (ii) The assumption of *weak-coupling*. Here, the standard condition from perturbation theory, $\|V\|_\infty \ll \text{gaps}(H)$, is not sufficient in the thermodynamic limit, due to the fast growth of the density of states and the corresponding shrinking of the gaps in the system size. Instead, it is replaced with a physically relevant condition, $\|V\|_\infty \ll k_B T$, which is robust in the thermodynamic limit.
(iii) An assumption about the *density of states* of the bath[5], namely, that it grows faster than exponentially with the energy and that it can be locally approximated by an exponential.

Note that the weak-coupling condition will not be satisfied in spatial dimensions higher than one for sufficiently large subsystems, since the interaction strength typically scales as the boundary of the subsystem S. This will be the case regardless of the strength of the coupling per particle or the relative size between S and B. This should not be seen as a deficiency of the above results, but as a feature of strong interactions. Systems that strongly interact with their environment do not in general equilibrate towards a Gibbs state, in a similar way that the reduced state (of a part) of a Gibbs state need not have Gibbs form [57, 58]. In this context, the findings of [59] suggest that subsystems do not relax towards a local Gibbs state but to the reduction of the global Gibbs state; this is shown for translation-invariant quantum lattices with finite range but arbitrarily strong interactions. The *eigenstate thermalization hypothesis* (ETH) [60, 61] gives further substance to this expectation. ETH has several formulations. Its simplest one is maybe the one introduced in [61]. It states that the expectation value $\langle E_k | O | E_k \rangle$ of a few-body observable O in an individual Hamiltonian eigenstate $|E_k\rangle$ equals

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[5] The density of states of the bath $\varrho^B(E)$ is the number of eigenstates of the bath with energy close to E.

the thermal average of O at the mean energy E_k. Although ETH has been observed for some models, it is not true in general and it is well known to break down for integrable models (see [61] for an example with hard-core bosons and references in [28] for further examples).

In the same spirit, it has recently been proven that a global microcanonical state (the completely mixed state of a energy shell subspace spanned by the Hamiltonian eigenstates with energy inside a narrow interval) and a global Gibbs state are locally indistinguishable for short range spin Hamiltonians off criticality, that is, when they have a finite correlation length [62]. This represents a rigorous proof of the so called *equivalence of ensembles*. If the Hamiltonian is not translationally invariant, the local indistinguishability between canonical and microcanonical ensembles becomes a typical property of the subsystems, allowing for rare counterexamples.

Concerning the latter condition on the density of states of the bath, in [63] it has been proven that the density of states of translational invariant spin chains tends to a Gaussian in the thermodynamic limit, matching the suited property of being well approximated by an exponential. In [62], the same statement is proven for any short ranged spin Hamiltonian.

Let us finally point out that not all systems thermalize. For instance, *integrable systems* are not well described by the Gibbs ensemble. This is due to the existence of local integrals of motion, i.e. conserved quantities, Q_α that keep the memory about the initial state. Instead, they turn to be described by the generalized Gibbs ensemble (GGE) defined as

$$\tau_{\mathrm{GGE}} \propto \exp\left(-\beta\left(H + \sum_\alpha \mu_\alpha Q_\alpha\right)\right), \tag{7}$$

where the generalized chemical potential μ_α is a Lagrange multiplier associated to the conserved quantity Q_α such that its expectation value is the same as the one of the initial state. The GGE was introduced by Jaynes in [17] where he pointed out that statistical physics can be seen as statistical inference and an ensemble as the least biased estimate possible on the given information. Nevertheless, note that any system has as many conserved quantities as the dimension of the Hilbert space, e.g. $Q_\alpha = |E_\alpha\rangle\langle E_\alpha|$. If one includes all these conserved quantities into the GGE the ensemble obtained is the diagonal ensemble introduced in equation (4). Note that the description of the equilibrium state by the diagonal ensemble requires the specification of as many conserved quantities as the dimension of the Hilbert space, which scales exponentially in the system size, and becomes highly inefficient. A question arises here naturally, is it possible to provide an accurate description of the equilibrium state specifying only a polynomial number of conserved quantities? If so, what are these *relevant conserved quantities* Q_α that allow for an accurate and efficient representation of the ensemble? This question is tackled in [64]. There, it is argued that the relevant conserved quantities are the ones that make the GGE as close as possible to the diagonal ensemble in the relative entropy distance $D(\omega\|\tau_{\mathrm{GGE}})$, which in this particular case can be written as

$$D(\omega\|\tau_{\mathrm{GGE}}) = S(\tau_{\mathrm{GGE}}) - S(\omega), \tag{8}$$

where we have used that the diagonal ensemble and the GGE have by construction the same expectation values for the set of selected conserved quantities, i.e. $\mathrm{Tr}(Q_\alpha \tau_{\mathrm{GGE}}) = \mathrm{Tr}(Q_\alpha \omega)$. Equation (8) tells us that the relevant conserved quantities are the ones the minimize the entropy $S(\tau_{\mathrm{GGE}})$. Note that in contrast to Jaynes approach, where entropy is maximized for a set of observables defined beforehand, here the notion of physically relevant is provided by how much an observable is able to reduce the entropy by being added into the set of observables that defines the GGE.

If instead of calculating the relative entropy between the diagonal ensemble and the GGE's we do it with respect to the set of product states, i.e.

$$T(\omega) := \min_{\pi_1, \pi_2, \ldots, \pi_n} D(\omega \| \pi_1 \otimes \pi_2 \otimes \ldots \pi_n), \tag{9}$$

then we obtain a measure of the *total (multipartite) correlations* of the diagonal ensemble. In [65] the scaling with system size of the total correlations of the diagonal ensemble has been shown to be connected to ergodicity breaking and used to investigate the phenomenon of many-body localization.

2.4. Equilibration times

Maybe the major challenge that is still open in the equilibration problem is to determine the equilibration timescale. It turns out that even if we know that a system equilibrates, there are no relevant bounds on how long the equilibration process takes. There could be quantum systems that are going to equilibrate, but whose equilibration times are of the order of magnitude of the age of the Universe, or alternatively, some systems, like glasses, which do not relax to equilibrium at all, but have metastable states with long lifetimes. The problem of estimating equilibration timescales is thus essential in order to have a full understanding of thermalization.

So far, progress on this issue has taken place from two different approaches. On the one hand, rigorous and completely general bounds on equilibration times have been presented in [51]. Due to their generality, these bounds scale exponentially with the system size, leading to equilibration times of the age of the Universe for macroscopic systems. On the other hand, very short equilibration times have been proven for generic observables [66], Hamiltonians [67–71], and initial states [72]. In nature, systems seem to equilibrate in a time that is neither microscopic nor exponential in the system size. A relevant open question is what properties of the Hamiltonians and operators lead to reasonable equilibration time. As a first step, in [73], a link between the complexity of the Hamiltonian's eigenvectors and equilibration time is presented. The result does not completely solve the question, since the given bounds are not fulfilled by all Hamiltonians but only by a fraction of them, and further research in this direction is needed.

2.5. Outlook

The aim of this section has been to justify that thermal states emerge in Nature for generic Hamiltonians. To complete the picture presented here we recommend the article [28] where an extensive review of the literature on foundations of statistical mechanics is provided.

The main ideas presented here have also been widely studied in the context of condensed matter physics, in which systems are typically brought out of equilibrium by sudden (and slow) *quantum quenches*: the Hamiltonian of a system (that is initially in the ground state) is suddenly (or smoothly) changed in time. We recommend the review article [29] on non-equilibrium dynamics of closed interacting quantum systems.

Let us finish the section with a list of some of the open problems that we consider most relevant in the field:

- *Typicality for symmetric states*. Hamiltonians in nature are not generic but have symmetries. Hence, the notion of typicality should be extended to physical states that are produced by symmetric Hamiltonians.
- *Quantum notion of integrability*. One of the reasons why it is so difficult to extract strong statements on the equilibration and thermalization of many body quantum systems is the

absence of a satisfactory quantum notion of integrability [74]. This leads first to some widespread confusion, since integrability is mentioned very often in the field of non-equilibrium dynamics, and second it does not allow us to classify quantum systems into classes with drastically different physical behaviour, like what occurs in classical mechanics.

- *Equilibration times*. Without bounds on the equilibration time scales, statements on equilibration become useless. As we have seen, the equilibration times are model dependent. We need then to understand how the equilibration times depend on the features of the Hamiltonian and the set of observables considered.
- *Relative thermalization*. It was highlighted in [75] that local thermalization of a subsystem S, as described here, is not enough to guarantee that S will act as thermal bath towards another physical system R. In other words, imagine that we want to perform quantum thermodynamics on a reference system R, using S as a thermal bath. To model a thermodynamic resource theory that recovers the laws of thermodynamics, it is not sufficient to demand that S be in a local Gibbs state $\tau_S(\beta)$. Indeed we need S to be thermalized relative to R, that is the the two systems should be uncorrelated, in global state, $\tau_S(\beta) \otimes \rho_R$. If this does not hold, then we cannot recover the usual thermodynamic monotones (for instance, there could be anomalous heat flows against the temperature gradient). Therefore, the relevant question for resource theories of thermodynamics is not only 'does S thermalize locally after evolving together with an environment?', but rather 'does S thermalize relative to R after evolving together with an environment?', and the results discussed in this section should be generalized to that setting. First steps in this direction can be found in [75], where the authors use decoupling—a tool developed in quantum information theory to find initial conditions on the entropies of the initial state that lead to relative thermalization.

3. Resource theories

In the previous section we reviewed recent progress in understanding how systems come to equilibrium, and in particular thermal equilibrium. We will now take thermalization as a given, and in the remaining of this review we explore the thermodynamics of quantum systems that interact with thermal states. We will start from an operational point of view, treating the thermal state as a 'free resource', a view inspired by other resource theories from quantum information.

In this section we discuss the approach of thermodynamics as a resource theory in more detail. Let us start by introducing the basic ideas behind resource theories that can be found in the literature, entanglement theory being the paradigmatic example. The first step is to fix the *state space S*, which is usually compatible with a composition operation—for instance, quantum states together with the tensor product, in systems with fixed Hamiltonians. The next step is to define the set of *allowed state transformations*. For thermodynamics, these try to model adiabatic or isothermal operations—like energy-preserving reversible operations, and contact with a heat bath.

The set of allowed operations induces a structure on the state space: we say that $\rho \to \sigma$ if there is an allowed transformation from ρ to σ. The relation $\to$ is a *pre-order*, that is, a binary relation that is both reflexive ($\rho \to \sigma$) and transitive ($\rho \to \sigma$ and $\sigma \to \tau$ implies $\rho \to \tau$; this results from composing operations one after the other).

The task now is to find general properties of this structure. A paradigmatic example is looking for simple necessary and sufficient conditions for state transformations. The most general case are functions such that

- $\rho \rightarrow \sigma \Rightarrow f(\rho, \sigma) \geqslant 0$ (that is, $f(\rho, \sigma) \geqslant 0$ is a *necessary* condition for state transformations), or
- $f(\rho, \sigma) \geqslant 0 \Rightarrow \rho \rightarrow \sigma$ (that is, $f(\rho, \sigma) \geqslant 0$ is a *sufficient* condition for state transformations).

Often, we try to find necessary and sufficient conditions as functions that can be written like $f(\rho, \sigma) = g(\rho) - h(\sigma)$. In the special case where $g = h$ for a necessary condition $(\rho \rightarrow \sigma \Rightarrow g(\rho) \geqslant g(\sigma))$, we call g a *monotone* of the resource theory. For example, in classical, large-scale thermodynamics, the free energy is a monotone.

In order to quantify the cost of state transformations, we often fix a minimal unit in terms of a *standard resource* that can be composed. For example, in entanglement theory the standard resource could be a pair of maximally entangled qubits, and in quantum thermodynamics we could take a single qubit (with a fixed Hamiltonian) in a pure state. The question then is 'how many pure qubits do I need to append to ρ in order to transform it into σ?' or, more generally, 'what is the cost or gain, in terms of this standard resource, of the transformation $\rho \rightarrow \sigma$?' [76–78].

One may also try to identify special sets of states. The most immediate one would be the set of *free states*: those that are always reachable, independently of the initial state. In standard thermodynamics, these tend to be what we call equilibrium states, like Gibbs states. Another interesting set is that of *catalysts*, states that can be repeatedly used to aid in transformations. We will revisit them shortly.

3.1. Models for thermodynamics

Now that we have established the basic premise and structure of resource theories, we may look at different models for resource theories of thermodynamics, which vary mostly on the set of allowed operations. In the good 'spherical cow' tradition of physics, the trend has been to start from a very simple model that we can understand, and slowly expand it to reflect more realistic scenarios. In general there are two types of operations allowed: contact with a thermal bath and reversible operations that preserve some thermodynamic quantities. Each of those may come in different flavours.

3.1.1. Noisy and unital operations. In the simplest case, all Hamiltonians are fully degenerate, so thermal states of any temperature are just fully mixed states, and there are no special conserved quantities. In this setting, thermodynamics inherits directly from the theory of noisy operations [79]. We may model contact with a thermal bath as composition with any system in a fully mixed state, and reversible operations as any unitary operation. Furthermore, we assume that we can ignore, or trace out, any subsystem. Summing up, noisy operations have the form

$$\mathcal{T}(\rho_A) = \mathrm{tr}_{A'}\left(U_{AB}\left[\rho_A \otimes \frac{\mathbb{1}_B}{|B|}\right]U_{AB}^\dagger\right),$$

where A' is any subsystem of AB and U is a unitary matrix. Alternatively, we may allow only for maps that preserve the fully mixed state, $\mathcal{T}_{A \rightarrow B} : \mathcal{T}_{A \rightarrow B}\left(\frac{\mathbb{1}_A}{|A|}\right) = \frac{\mathbb{1}_B}{|B|}$, called *unital maps* (an example would be applying one of two isometries and then forgetting which one). The

two sets—noisy operations and unital maps—induce the same pre-order structure in the state space. In this setting, *majorization* is a necessary and sufficient condition for state transformations [79]. Roughly speaking, majorization tells us which state is the most mixed. Formally, let $\mathbf{r} = (r_1, r_2, ..., r_N)$ and $\mathbf{s} = (s_1, s_2, ..., s_N)$ be the eigenvalues of two states ρ and σ respectively, in decreasing order. We say that $\mathbf{r}$ majorizes $\mathbf{s}$ if $\sum_{i=1}^{k} r_i \geqslant \sum_{i=1}^{k} s_i$, for any $k \leqslant N$. In that case $\rho \rightarrow \sigma$; monotones for this setting are called *Schur monotone functions*, of which information-theoretical entropy measures are examples [78, 80–83]. For example, if ρ majorizes σ, then the von Neumann entropy of ρ, $S(\rho) = -\mathrm{tr}(\rho \log_2 \rho)$, is smaller than $S(\sigma)$. For a review, see [83].

3.1.2. Thermal operations. The next step in complexity is to let systems have non-degenerate Hamiltonians. The conserved quantity is energy, and equilibrium states are Gibbs states of a fixed temperature T. For instance for a system A with Hamiltonian H_A, the equilibrium state is $\tau_A(\beta) = \mathrm{e}^{-\beta H_A}/\mathcal{Z}$. We can model contact with a heat bath as adding any system in a Gibbs state—this corresponds to the idealization of letting an ancilla equilibrate for a long time. A first approach to model physical reversible transformations is to allow for unitary operations U that preserve energy—either absolutely ($[U, H] = 0$) or on average ($\mathrm{tr}(H\rho) = \mathrm{tr}(H\,(U\rho U^\dagger))$ for specific states). Finally, we are again allowed to forget, or trace out, any subsystem. Together, these transformations are called thermal operations,

$$\mathcal{T}(\rho_A) = \mathrm{tr}_{A'}(U_{AB}[\rho_A \otimes \tau_B(\beta)]U_{AB}^\dagger),$$

where A' is any subsystem of AB and U is an energy-conserving unitary [84]. The monotones found so far are different versions of the free energy, depending on the exact regime [82, 85–88] (see example 1). It is worth mentioning we can build necessary conditions for state transformations from these monotones, but sufficiency results are only known for classical states (states that are block-diagonal in the energy eigenbasis) [82] and any state of a single qubit [89, 90]. In the limit of a fully degenerate Hamiltonian, we recover the resource theory of noisy operations.

Example 1. Free energy as a monotone. This is an example of finding monotones for the resource theory of thermal operations [85]. We are interested in finding the optimal rates of conversion between two states ρ and σ, in the limit of many independent copies

$$R(\rho \rightarrow \sigma) := \sup_R \lim_{n \rightarrow \infty} \rho^{\otimes n} \rightarrow \sigma^{\otimes Rn}.$$

If both $R(\rho \rightarrow \sigma)$, $R(\sigma \rightarrow \rho) > 0$, and these quantities represent optimal conversion rates, then the process must be reversible, that is, $R(\rho \rightarrow \sigma) = 1/R(\sigma \rightarrow \rho)$; otherwise we could build a perpetual motion engine, and the resource theory would be trivial. The idea is to use a minimal, scalable resource α as an intermediate step. We can think of α as a currency: we will sell n copies of ρ for a number of coins, and use them to buy some copies of σ. To formalize this idea, we define the selling and buying cost of a state ρ, or more precisely the distillation and formation rates

$$R^D(\rho) := R(\rho \rightarrow \alpha), \qquad R^F(\rho) := R(\alpha \rightarrow \rho) = \frac{1}{R^D(\rho)}.$$

In the optimal limit we have the process

$$\rho^n \rightarrow \alpha^{nR^D(\rho)} \rightarrow \sigma^{nR^D(\rho)R^F(\sigma)} \iff \rho^n \rightarrow \sigma^{nR(\rho \rightarrow \sigma)},$$

which gives us the relation

$$R(\rho \to \sigma) = \frac{R^D(\rho)}{R^D(\sigma)}.$$

We have reduced the question to finding the distillation rate, which depends on the choice of α. For example, take ρ, σ and α to be classical states (diagonal in the energy basis) of a qubit with Hamiltonian $H = \Delta |1\rangle\langle 1|$. For the currency, we choose $\alpha = |1\rangle\langle 1|$. The distillation rate is found by use of information-compression tools [85]. It is given by the relative entropy between ρ and the thermal state $\tau(\beta)$,

$$\begin{aligned}R^D(\rho) &= D(\rho \| \tau(\beta))\\ &= \mathrm{tr}(\rho(\log \rho - \log \tau(\beta)))\\ &= \beta(F_\beta(\rho) - F_\beta(\tau(\beta))),\end{aligned}$$

where $F_\beta(\rho) = \langle E \rangle_\rho - \beta^{-1} S(\rho)$ is the free energy of ρ at inverse temperature β. All in all, we find the conversion rate

$$R(\rho \to \sigma) = \frac{F_\beta(\rho) - F_\beta(\tau(\beta))}{F_\beta(\sigma) - F_\beta(\tau(\beta))}.$$

Now we can apply this result to find a monotone for a single-shot scenario: in order to have $\rho \to \sigma$ we need in particular that $R(\rho \to \sigma) \geqslant 1$. In other words, we require $F_\beta(\rho) \geqslant F_\beta(\rho)$, thus recovering the free energy as a monotone for the resource theory of thermal operations. If we work directly in the single-shot regime, we recover a whole family of monotones [82] based on quantum Rényi relative entropies [91], of which the free energy is a member.

3.1.3. Gibbs-preserving maps. Following the example of the theory of noisy operations, we could try to replace these thermal operations with so-called Gibbs-preserving maps, that is, maps such that $\mathcal{T}_{A \to B}(\tau_A(\beta)) = \tau_B(\beta)$. This constraint is easier to tackle mathematically, and the two resource theories induce the same pre-order on classical states, leading to a condition for state transformation called Gibbs-majorization (which is majorization after a rescaling of the eigenvalues) [87]. However, Gibbs-preserving maps are less restrictive than thermal operations for general quantum states [92]. For example, suppose that you have a qubit with the Hamiltonian $H = E |1\rangle\langle 1|$, and you want to perform the transformation $|1\rangle \to |+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. This is impossible through thermal operations, which cannot create coherence; yet there exists a Gibbs-preserving map that achieves the task. We may still use Gibbs-preserving maps to find lower bounds on performance, but at the moment we cannot rely on them for achievability results, as they are not operationally defined.

3.1.4. Coherence. The difference between thermal operations and Gibbs-preserving maps is not the only surprise that quantum coherence had in store for thermodynamics enthusiasts. The question of how to create coherence in the first place led to an intriguing discovery. In order to achieve the above transformation $|1\rangle \to |+\rangle$ through thermal operations, we need to draw coherence from a reservoir. A simple example of a coherence reservoir would be a doubly infinite harmonic oscillator, $H = \sum_{n=-\infty}^{\infty} n\Delta |n\rangle\langle n|$, in a coherent state like $|\Psi\rangle = N^{-1}\sum_{n=a}^{a+N} |n\rangle$. Lasers approximate such reservoirs, which explains why we can use them to apply arbitrary transformations on quantum systems like ion traps. One may ask what happens to the reservoir after the transformation: how much coherence is used up? Can we use the same reservoir to perform a similar operation in a new system? The unexpected answer is that coherence is, in a sense, catalytic: while the state of the reservoir is affected, its

ability to implement coherent operations is not [93]. What happens is that the state of the reservoir 'spreads out' a little with each use, but the property that determines the efficacy of the reservoir to implement operations stays invariant. In more realistic models for coherence reservoirs, where the Hamiltonian of the reservoir has a ground state, the catalytic properties hold for some iterations, until the state spreads all the way down to the ground state. At that stage, the reservoir needs to be recharged with energy to pump up the state again. Crucially, we do not need to supply additional coherence. In the converse direction, we know that coherence reservoirs only are critical in the single-shot regime of small systems. Indeed, in the limit of processing many copies of a state simultaneously, the work yields of doing it with and without access to a coherence reservoir converge [94].

3.1.5. Catalysts. The catalytic nature of coherence raises more general questions about catalysts in thermodynamics. Imagine that we want to perform a transformation $\rho \to \sigma$ in a system S, and we have access to an arbitrary ancilla in any desired state γ. Now suppose that our constraint is that we should return the ancilla in a state that is ϵ-close to γ:

$$\rho_S \otimes \gamma_A \to \sigma_{SA} : \qquad \|\sigma_A - \gamma_A\|_1 \leqslant \epsilon.$$

The question is whether we can overcome the usual limits found in thermal operations by use of this catalyst. In other words, can we perform the above transformation in cases where $\rho \to \sigma$ would not be allowed? It turns out that if no other restrictions are imposed on the catalyst, then for any finite ϵ and any two states ρ and σ, we can always find a (very large) catalyst that does the job [82]. These catalysts are the thermodynamic equivalent of embezzling states in LOCC [95]. However, if we impose reasonable energy and dimension restrictions on the catalyst, we recover familiar monotones for state transformations [82, 96]. These restrictions and optimal catalysts result from adapting the concept of trumping relations on embezzling states [97, 98] to the thermodynamic setting. In particular, if we demand that $\epsilon \propto n^{-1}$, where n is the number of qubits in the catalyst, we recover the free energy constraint for state transformations [96]. A relevant open question, motivated by the findings of catalytic coherence, is what happens if we impose operational constraints on the final state of the catalyst. That is, instead of asking that it be returned ϵ-close to γ, according to the trace distance, we may instead impose that its catalytic properties stay unaffected. It would be interesting to see if we recover similar conditions for allowed transformations under these constraints.

3.1.6. Clocks. All of resource theories mentioned allow for energy-preserving unitary operations to be applied for free. That is only the 'first order' approach towards an accurate theory of thermodynamics, though. Actually, in order to implement a unitary operation, we need to apply a time-dependent Hamiltonian to the systems involved. To control that Hamiltonian, we require very precise time-keeping—in other words, precise clocks, and we should account for the work cost of using such clocks. Furthermore, clocks are clearly out of equilibrium, and using them adds a source of free energy to our systems. Including them explicitly in a framework for work extraction forces us to account for changes in their state, and ensures that we do not cheat by degrading a clock and drawing its free energy. First steps in this direction can be found in [66]. There, the goal is to implement a unitary transformation in a system S, using a time-independent Hamiltonian. For this, the authors introduce an explicit clock system C hat runs continuously, as well as a weight W that acts as energy and coherence reservoir. The global system evolves under a time-independent Hamiltonian, designed such that the Hamiltonian applied on S depends on the position of the clock—which effectively measures time. The authors show that such a construction allows us to

approximately implement any unitary operation on S, while still obeying the first and second laws of thermodynamics. Furthermore, the clock and the weight are not degraded by the procedure (just like for catalytic coherence). In particular, this result supports the idea behind the framework of thermal operations: that energy-conserving unitaries can approximately be implemented for free (if we neglect the informational cost of designing the global Hamiltonian). Note that this is still an idealized scenario, in which the clock is infinite-dimensional and moves like a relativistic particle (the Hamiltonian is proportional to the particle's momentum). A relevant open question is whether there exist realistic systems with the properties assigned to this clock, or alternatively how to adapt the protocol to the behaviour of known, realistic clocks. That direction of research can be related to the resource theory of quantum reference frames [89, 99–101]. An alternative direction would be to ask what happens if we do not have a clock at all—can we extract all the work from a quantum state if we are only allowed weak thermal contact? This question is studied (and answered in the negative, for general states) in [102].

Example 2.   Heat engines. The extreme case where one of our resources is in itself a second heat bath is of particular interest. This is a very natural scenario in traditional thermodynamics: steam engines used a furnace to heat a chamber, and exploit the temperature difference to the cooler environment. The study of this limit led to landmark findings like trains, fridges and general heat engines, and to theoretical results on the efficiency of such engines. One might wonder whether these findings can also be applied at the quantum scale, and especially to very small systems composed only of a couple of qubits [25, 103]. The answer is yes: not only is it possible to build two-qubit heat engines, but they achieve Carnot efficiency [104, 105]. It is possible to build heat engines that do not require a precise control of interactions, in other words, that do not require a clock [104, 106].

3.1.7. Free states and passivity.   It is now time to question the other assumption behind the framework of thermal operations: that Gibbs states come for free. There are two main arguments to support it: firstly, Gibbs states occur naturally under standard conditions, and therefore are easy to come by; secondly, they are useless on their own. The first point, typicality of Gibbs states, is essentially the fundamental postulate of statistical mechanics: systems equilibrate to thermal states of Gibbs form. This assumption is discussed and ultimately justified from first principles in section 3. The second point is more subtle. Pusz and Woronowicz first introduced the notion of passive states, now adapted to the following setting [107–109]. Let S be a system with a fixed Hamiltonian H, in initial state ρ. We ask whether there is a unitary U that decreases the energy of S, that is

$$\mathrm{tr}(\rho H) > \mathrm{tr}(U\rho U^\dagger H).$$

If we can find such a unitary, then we could extract work from S by applying U and storing the energy difference in a weight system. If there is no U that achieves the condition above, then we cannot extract energy from ρ, and we say that the state is *passive*. The latter applies to classical states (i.e., diagonal in the energy basis) whose eigenvalues do not increase with energy. However, suppose that now we allow for an arbitrary number n many copies of ρ and a global unitary U_{gl}. The question becomes whether

$$\mathrm{tr}(\rho H) > \frac{1}{n}\mathrm{tr}(U_{\mathrm{gl}}\ \rho^{\otimes n}\ U_{\mathrm{gl}}^\dagger\ H_{\mathrm{gl}}),$$

where H_{gl} is the global Hamiltonian, which is the sum of the independent local Hamiltonians of every system. If this is not possible for any n, we say that ρ is *completely passive*, and it

turns out that only states of Gibbs form, $\rho = \tau(\beta)$ are completely passive. Moreover, Gibbs states are still completely passive if we allow each of the n subsystems to have a different Hamiltonian, as long as all the states correspond to the same inverse temperature β. This justifies the assumption that we may bring in any number and shape of subsystems in thermal states for free, because we could never extract work from them alone—another resource is necessary, precisely a state out of equilibrium. More formally, it was shown that if a resource theory allows only for energy-conserving unitaries and composition with some choice of free states, Gibbs states are the only choice that does not trivialize the theory [82, 110].

3.1.8. Different baths. The results outlined above suggest that thermodynamics can be treated as information processing under conservation laws, and so researchers began to experiment with other conserved quantities, like angular momentum [111–113], using the principle of maximum entropy to model thermal momentum baths. The state of those baths has again an exponential Gibbs form, with operators like L replacing H. The same type of monotones emerged, and similar behaviour was found for more general conserved quantities [110, 114].

3.1.9. Finite-size effects. Another setting of practical interest is when we have access to a heat bath but may not draw arbitrary thermal subsystems from it. For instance, maybe we cannot create systems with a very large energy gap, or we can only thermalize a fixed number of qubits. In this case, the precision of state transformations is affected, as shown in [115], and we obtain effective measures of work cost that converge to the usual quantities in the limit of a large bath. The opposite limit, in which all resources are large heat baths, leads to the idea of heat engines (example 2).

3.1.10. Single-shot regime. Some of the studies mentioned so far characterize the limit of many independent repetitions of physical experiments, and quantify things like the average work cost of transformations or conversion rates [85, 94]. The monotones found (like the von Neumann entropy and the usual free energy) are familiar from traditional thermodynamics, because this regime approximates the behaviour of large uncorrelated systems. As we move towards a thermodynamic theory of individual quantum systems, it becomes increasingly relevant to work in the single-shot regime. Some studies consider exact state transformations [76, 77, 113], while others allow for a small error tolerance [78, 80, 81, 86, 87, 110, 114, 116, 117]. The monotones recovered correspond to operational entropy measures, like the smooth max-entropy (see example 3), and variations of a single-shot free energy that depend on the conservation laws of the setting; in general, they can be derived from quantum Rényi relative entropies [91] between the initial state and an equilibrium state [82, 118]. Single-shot results converge asymptotically to the traditional ones in the limit of many independent copies. The relation between single-shot and average regimes is studied via fluctuation theorems in [119].

3.1.11. Definitions of work. In classical thermodynamics, we can define work as some form of potential energy of an external device, which can be stored for later use. For instance, if a thermodynamic process results in the expansion of a gas against a piston, we can attach that piston to a weight, that is lifted as the gas expands. We count the gain in gravitational potential energy as work—it is well-ordered energy that can later be converted into other forms, according to the needs of an agent. A critical aspect is that at this scale fluctuations are negligible, compared to the average energy gain. In the regime of small quantum systems, this no longer holds, and it is not straightforward to find a good definition of work. Without a

framework for resource theories of thermodynamics, a system for work storage is often left implicit. One option is to assume that we can perform any joint unitary operation U_{SB} in a system S and a thermal bath B, and work is defined as the change in energy in the two systems manipulated, $W := \text{tr}(H_{SB}\,\rho_{SB}) - \text{tr}(H_{SB}\,U_{SB}\,\rho_{SB}\,U_{SB}^{\dagger})$, where H_{SB} is the (fixed) Hamiltonian of system and bath, and ρ_{SB} the initial state [115]. Another example, inheriting more directly from classical thermodynamics, assumes that we can change the Hamiltonian of S and bring it in contact with an implicit heat bath [120]; work at a time t is then defined as

$$W(t) := \int_0^t \mathrm{d}t'\,\text{tr}\!\left(\rho_S(t')\frac{\mathrm{d}H_S(t')}{\mathrm{d}t'}\right).$$

To study fluctuations around this average value, we consider work to be a random variable in the single-shot setting—this is explored in section 6. Note that in these examples work is not operationally motivated; rather it is defined as the change of energy that heat cannot account for. Resource theories of thermodynamics, with their conservation laws, force us to consider an explicit system W for work storage. We act globally on $S \otimes W$, and we can define work in terms of properties of the reduced state of W. One proposal for the quantum equivalent of a weight that can be lifted, for the resource theory of thermal operations, is a harmonic oscillator, with a regular Hamiltonian $H_W = \sum_n n\,\epsilon\,|n\rangle\langle n|$. The energy gaps need to be sufficiently small to be compatible with the Hamiltonian of S; in the limit $\epsilon \to 0$ the Hamiltonian becomes $H_W = \int \mathrm{d}x\, x\, |x\rangle\langle x|$ [86, 105]. Average work is defined as $\text{tr}(H_W\,\rho_W^{\text{final}}) - \text{tr}(H_W\,\rho_W^{\text{initial}})$, and fluctuations can be studied directly in the final state of the work storage system, ρ_W. This approach also allows us to observe other effects, such as the build up of coherences in W, and of correlations between W and S. Another advantage is that we can adapt the storage system to other resource theories: for instance, we can have an angular momentum reservoir composed of many spins, and count work in terms of polarization of the reservoir [112]. These approaches are critically analysed in [121]; in particular, it is highlighted that some do not distinguish work from heat. For instance, thermalizing the work storage system may result in an increase of average energy, which is indiscriminately labelled as 'average work'. In the same paper, an axiomatic approach to define work is proposed, based onconcepts from resource theories and interactive proofs. There, work is seen as a figure of merit: a real function assigned to state transformations, $\mathcal{W}(\rho \to \sigma)$. Starting from a couple of assumptions, the authors derive properties of acceptable work functions $\mathcal{W}$: for instance, that they can be written as the difference between a monotone for initial and final state, $\mathcal{W}(\rho \to \sigma) = g(\rho) - g(\sigma)$. The free energy is an example of such a valid work function.

Example 3. Landauer's principle. How much energy is needed to perform logical operations? What are the ultimate limits for heat dissipation of computers? These questions lie at the interface between thermodynamics and information theory, are of both foundational and practical interest. As Bennett realized, all computations can be decomposed into reversible operations followed by the erasure of a subsystem [122]. If we assume that the physical support of our computer is degenerate in energy, we recover the setting of noisy operations, in which unitaries are applied for free. That way, the thermodynamic cost of computation is simply the cost of erasure, which is defined as taking a system from its initial state ρ to a standard, predefined pure state $|0\rangle$ (like when we format a hard drive). Rolf Landauer first proposed that the work cost of erasing a completely unknown bit of information (think of a fully mixed qubit) in an environment of temperature T is $k_B T \ln 2$ [12]. That very same limit was also found for quantum systems, in the setting of thermal operations

[115, 123], for the ideal case of an infinitely large heat bath and many operations; finite-size effects are analysed in [115].

Using Landauer's principle as a building block, we can approach the more general question of erasing of a system that is not in a completely unknown state, but rather about which we have partial information. For example, imagine that we want to perform an algorithm in our quantum computer, and then erase a subsystem S (which could be a register or ancilla). The rest of our computer may be correlated with S, and therefore we can use it as a memory M, and use those correlations to optimize the erasure of S. In short, we want to take the initial state ρ_{SM} to $|0\rangle\langle0|_S \otimes \rho_M$, erasing S but not disturbing M. It was shown [78, 81] that the optimal work cost of that transformation is approximately $H_{\max}^\epsilon(S|M)_\rho k_B T \ln 2$, where ϵ parametrizes our error tolerance and $H_{\max}^\epsilon(S|M)_\rho$ is the smooth max entropy, a conditional entropy measure that measures our uncertainty about the state of S, given access to the memory M. It converges to the von Neumann entropy in the limit of many independent copies. In the special case where S and M are entangled, it may become negative—meaning that we may gain work in erasure, at the cost of correlations. Not incidentally, these results use quantum information processing techniques to compress the correlations between S and M before erasure; after all, 'information is physical' [124].

3.2. Generalizing resource theories

Let us now abstract from particular resource theories, and think about their common features, and how we may generalize them.

3.2.1. Starting from the pre-order. As mentioned before, the set of allowed transformations imposes a pre-order structure $(S, \leqslant)$ on the state space S. One direction towards exploring the concept of resource theories could be to start precisely from such a pre-order structure. That was the approach of Carathéodory, then Giles and later Lieb and Yngvason, who pioneered the idea of resource theories for thermodynamics [76, 77, 125, 126]. In their work, the set of allowed transformations is implicitly assumed, but we work directly with an abstract state space equipped with a preorder relation. They were largely inspired by classical, macroscopic thermodynamics, as one may infer from the conditions imposed on the state space, but their results can be applied to thermodynamics of small quantum systems [113]. Assuming that there exist minimal resources that can be scaled arbitrarily and act as 'currency', the authors obtain monotones for exact, single-shot state transformations. When applied to the pre-order relation on classical states that emerges from thermal operations, these monotones become single-shot versions of the free energy [113].

3.2.2. Starting from the set of free resources. In [118] general quantum resource theories are characterized based on the set of free resources of each theory. Assuming that the set of free states is well-behaved (for instance, that it is convex, and that the composition of two free states is still a free state), they show that the relative entropy between a resource and the set of free states is a monotone. This is because the relative entropy is contractive (non-increasing under quantum operations); the same result applies to any contractive metric. Finally, they find an expression for the asymptotic value of a resource in terms of this monotone: the conversion rate between two resources is given by the ratio between their asymptotic value.

3.2.3. In category theory. Reference [16], and more recently [37] have generalized the framework of resource theories to objects known as symmetric monoidal categories. These can represent essentially any resource that can be composed (in the sense of combining copies

of different resources, like tensoring states in quantum theory). The authors consider both physical states and processes as possible resources. After obtaining the pre-order structure from a set of allowed operations, resource theories can be classified according to several parameters. For instance, the authors identify quantitative theories (where having more of a resource helps, like for thermal operations) and qualitative ones (where it helps to have many different resources). They find expressions for asymptotic conversion rates in different regimes and, crucially, give varied examples of resource theories, within and beyond quantum theory, showing just how general this concept is.

3.2.4. Resource theories of knowledge. In [127], emphasis is given to the subjective knowledge of an observer. The framework introduced there allows us to embed macroscopic descriptions of reality into microscopic ones, which in turn lets us switch between different agents' perspectives, and see how traditional large-scale thermodynamics can emerge from quantum resource theories like thermal operations. It also allows us to combine and relate different resource theories (like thermodynamics and LOCC), and to infer the structure of the state space (like the existence of subsystems or correlations) from modularity and commutativity of transformations.

3.3. Outlook

In the previous sections we identified several open problems. These can be grouped into two main directions:

- *Quantumness: coherence, catalysis and clocks.* It remains to find optimal coherent catalysts and clocks under realistic constraints (a generalization of [96]). This would give us a better understanding of the thermodynamic power and limitations of coherent quantum states. It would also allow us to account for all costs involved in state transformations.
- *Identifying realistic conditions.* We have been very good at defining sets of allowed transformations that are analogous to those of traditional thermodynamics, and recover the same monotones (like the free energy) in the limit of large, uncorrelated systems. The original spirit of thermodynamics, however, was to find transformations that were easy and cheap to implement for experimenters—for instance, those whose cost did not scale with the relevant parameters. In order to find meaningful resource theories for individual quantum systems, it is again imperative to turn to concrete experimental settings and try to identify easy and cheap transformations and resources. At this stage, it is not yet clear whether these will correspond to thermal operations, time-independent Hamiltonians, or another model of quantum thermodynamics—in fact it is possible that they vary depending on the experimental realization, from superconducting qubits to ion traps.

4. Entanglement theory in thermodynamic settings

In the previous sections we have established how quantum information can be used to understand the very foundation of thermodynamics, from the emergence of thermal states to the resource theory of manipulating these with energy conserving unitaries. We have seen that phrasing thermodynamics as a resource theory can elucidate the meaning of thermodynamic quantities at the quantum scale, and how techniques originally developed for a resource theory of communication can facilitate this endeavour. The motivation behind this approach is

a very practical one: finding the ultimate limitations of achievable transformations under restrictions that follow from the nature of the investigated system that naturally limits the set of operations we can perform. As quantum information processing is becoming increasingly applied, we also need to think about fundamental restrictions to quantum information itself, emerging from unavoidable thermodynamic considerations. There has thus been an increased interest in investigating scenarios of quantum information processing where thermodynamic considerations cannot be ignored. From fundamental limitations to the creation of QIP resources to their inherent work cost. In this section we try to give a brief overview over recent developments in this intersection with a focus on the paradigmatic resource of QIP: entanglement.

4.1. Correlations and entanglement under entropic restrictions

Entanglement theory is in itself one of the most prominent examples of resource theories. Entanglement, a resource behind almost all tasks in quantum information processing, is hard to create and once distributed can only decrease. Thus in entanglement theory classically correlated states come for free and local operations are considered cheap, which singles out entanglement as the resource to overcome such limitations. These limitations and resources are of course very different to the resources and tasks explored in the previous sections. A comprehensive comparison between the principles behind these and more general resource theories is made in [128] and as examples of a more abstract treatment in [16].

Such resource theories are always designed to reflect specific physical settings, such as LOCC [129] as a natural constraint for communication. It is therefore unavoidable that when describing various physical circumstances these resource theories can be combined yielding hybrid theories. One natural example is the desire to process quantum information in a thermodynamic background. Ignoring limitations coming from available energies in a first step this leads to the task of producing resources for computation (such as entanglement or correlation) at a given entropy. Some of the first considerations in this direction were motivated by the prospect of using nuclear magnetic resonance (NMR) for quantum computation. Due to non-zero temperature, i.e. non-trivial restrictions on the entropy of the state, such systems would always be fairly close to the maximally mixed state.

In this context the most natural question to ask, is whether a unitary transformation is capable of entangling a given input state. As a precursor to studying the possibility of entangling multipartite states, the complete solution for two qubits was found in [130] and later decent bounds on bipartite systems of arbitrary dimension were presented in [131].

Another pathway was pursued by [132–134], where with NMR quantum computation in mind, volumes of separable states around the maximally mixed state were identified. These volumes imply that if any initial state is in close proximity of the maximally mixed state, there can be no chance of ever creating entanglement in such states, as the distance from the maximally mixed state is invariant under unitary transformations. Further improvements in terms of limiting temperatures were obtained in [135].

The question of whether a given state can be entangled under certain entropy restrictions clearly relies only on the eigenvalue spectrum of the considered state, as the best conceivable operation creating entanglement is a unitary one (which leaves eigenvalues unchanged). These questions were further pursued under the name of 'separability from spectrum' in [136–138]. One of the main results important in the context of quantum thermodynamics is the following: a state with eigenvalues λ_i, ordered by size, i.e. $\{\lambda_i \geqslant \lambda_{i+1}\}$ can be entangled by an appropriate unitary if

$$\lambda_1 > \lambda_{d-1} + 2\sqrt{\lambda_{d-2}\lambda_d}. \tag{10}$$

More importantly, for $2 \times m$ dimensional states, this condition is not only sufficient, but also necessary [138].

Moving beyond the mere presence of entanglement in the unitary orbit of input states, one encounters an intrinsic difficulty of properly quantifying the entanglement created. There is a whole 'zoo' of entanglement measures [139, 140] and only in the bipartite case there is a unique 'currency' known, i.e. a paradigmatic resource state from which all other states can be created via LOCC (although recent progress has been made in the four qubit case, where it has been shown that after exclusion of a measure zero set, such a set of resource states can indeed be identified [141]).

In any case one can at least study general correlations with a clear operational interpretation, such as the mutual information, which has been performed in [142–144]. In these papers the authors have, among other things, identified minimally and maximally correlated states in the unitary orbit of bipartite systems. It turns out that at least here the entropy poses only a rather trivial restriction and for any d-dimensional state ρ a mutual information of $I_\rho(A : B) = 2\log_2(d) - S(\rho)$ can be achieved via global unitary rotations.

Exploiting these results [145] continued to study the generation of correlations and entanglement under entropic restrictions for multipartite systems. Inspired by the idea of thermal states as a free resource, the authors consider a multipartite system initially in a thermal state. They ask what is the highest temperature T_{ent} at which entanglement can still be created, it scales with the dimension of the partitions and quantify the inherent cost in terms average energy change (see example (4) for an exemplary two qubit energy cost). By introducing concrete protocols, i.e. unitary operations, the authors show that bipartite entanglement generation across all partitions of n-qubits is possible iff $k_B T/E < n/(2\ln(1 + \sqrt{2}))$ and genuine multipartite entanglement across all parties can be created if $k_B T/E < n/(2\ln(n)) + \mathcal{O}(n/\ln(n)^2)$.

4.2. Correlations and entanglement in a thermodynamic background

In the context of thermodynamics the previous subsection can be viewed as a very special case of operating on closed systems with an unlimited external energy supply or a fully degenerate Hamiltonian. As elaborated in section 4 of the review this does not encompass the whole potential of thermodynamic transformations. If the necessary correlating unitary does not conserve the total energy, we should account for the difference in average energy between initial and final states. Taking into account also the average energy cost reveals an intrinsic work value of correlations and entanglement in general. This fundamental fact was first quantified in [145]).

Example 4. Entangling two qubits. Creating entanglement from thermal states will always cost some energy. For the simplest case of entangling two qubits with energy gap E at zero temperature one can find a closed expression, e.g. for the concurrence, in terms of the invested average energy $\Delta E = W$:

$$C(W) = \sqrt{\frac{W}{E}\left(2 - \frac{W}{E}\right)}.$$

Accounting for the average energy change in the unitary orbit of initial quantum states however still does not encompass the whole potential of thermodynamic resource theories.

Thermal operations on target states can also make use of a thermal bath at temperature T and thus can also reduce the entropy of the target system. Disregarding energy costs in this context of course yields the rather trivial result that any quantum information processing resource can be produced, simply by cooling the system (close) to the ground state and then performing the adequate global unitary operation on it. Taking into account the free energy costs of correlating transformations, [146] has shown that every bit of correlation embodies an intrinsic work value proportional to the temperature of the system. For mutual information this yields a relation akin to Landauer's principle for the work cost of creating correlations W_{cor}

$$W_{\text{cor}} \geqslant k_{\text{B}}TI_{\rho}(A : B), \tag{11}$$

and it implies a general free energy cost of entanglement that is bounded from above and below for the bipartite case in [146]. All previous considerations are illustrated in figure 4.

That extractable work can be stored in correlations is by no means a purely quantum phenomenon. Even classical correlations can store work in situations where local work extraction is impossible. In [147] the quantum versus classical capacity for storing extractable work purely in correlations was compared. For two qubits twice as much work can be stored in entangled correlations as the best possible separable (or even classical, which turns out to be the same) correlations admit (a fact that is also mentioned in [75] in a different setting). However the difference between separably encoded work from correlations W_{sep} and the maximally possible work in correlations W_{max} scales as

$$\frac{W_{\text{sep}}}{W_{\text{max}}} = 1 - \mathcal{O}(n^{-1}), \tag{12}$$

i.e. the quantum advantage vanishes in the thermodynamic limit of large systems.

Concerning the extractable work from correlations one can also find seemingly contrary results if the figure of merit changes. The above considerations apply only if the target is an extraction of average energy or standard free energy, partially neglecting the details of the work distribution arising in the receiving system (detailed considerations of such work distribution fluctuations will be discussed in section 6). One can just as well be interested in a guaranteed amount of work. If that is the case one can arrive at more restrictions concerning work extraction as also recently demonstrated in [117]. Curiously in [148] it was shown, however, that these restrictions can be overcome by considering k initially uncorrelated catalysts that build up correlations in the process. In that context one can extract more deterministic work and can thus regard the stochastic independence of the input catalysts as a resource for work extraction, which is quite contrary to the case considered before and the thermodynamic limit.

A different, but very related, setting exploring work gain from correlations is studied in the context of quantum feedback control. Here the task is rather to quantify the inevitable work cost arising from information gain in the process of a measurement. As in order to measure a system one needs to correlate with the system in question it follows intuitively that this scenario will also always induce work cost related to bipartite correlations between the system and the memory storing the information gain about the system. Here the work cost coming purely from correlations was quantified in [144], building upon older results on the inevitable work cost of quantum measurements [149–152] and Landauer's principle. To model the necessary feedback control, the authors included a general model of a quantum memory upon which projective measurements can be performed. The authors also studied the possible work gain from bipartite quantum states in this context. Denoting the state of the memory as ρ_M the authors find an upper bound on the work gain (defined as the work

Two systems, initially in local, product thermal states of temperature T, are correlated using (a) any unitary [142], (b) a unitary changing the average energy by at most ΔE [144] or (c) a unitary on the systems and another bath at the same temperature T [145]. The local states of the two systems may heat up in the process: ΔT is infinite in (a), a function of ΔE in (b) and forced to be zero in (c). In general, for setting (b), the optimal conversion rate of average energy into mutual information is still unknown.
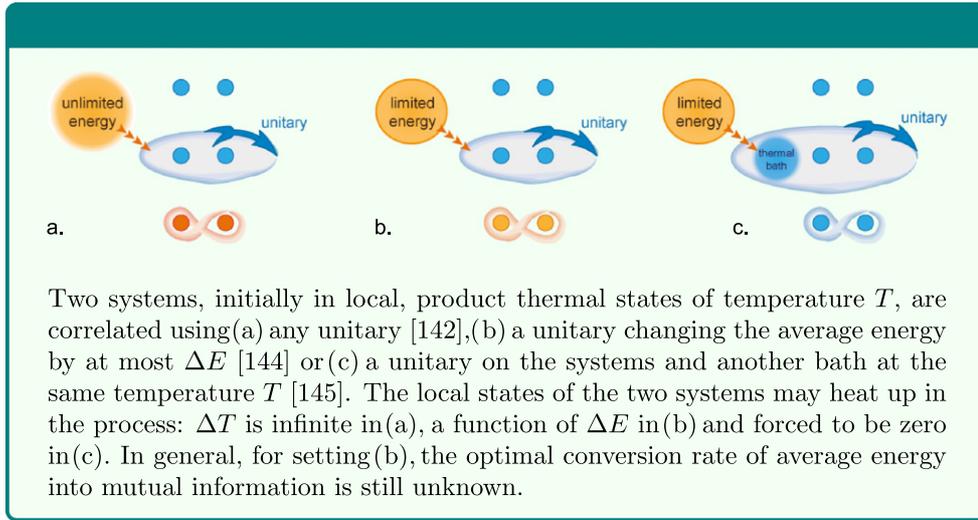
Figure 4. Creating correlations between local thermal states.

extracted from both subsystems minus the work cost of the measurements and subsequent erasure of the quantum memory) as

$$W_{\text{net}} \leqslant k_{\text{B}} T \left(I_\rho(A:B) - I_\rho(A:B|\rho_M) \right) - \Delta F_\beta(\rho). \tag{13}$$

4.3. Thermodynamics under locality restrictions

In the previous subsections we have reviewed the prospect of creating quantum information processing resources in a thermodynamic background. The other obvious connection between the resource theories of entanglement and thermodynamics is taking the converse approach. Here one is interested in thermodynamic operations under additional locality restrictions.

In [153] the difference between the extractable work from bipartite quantum states in thermodynamics both with and without locality restrictions was studied. The resulting difference, called the *work deficit*, can be bounded via

$$\Delta = \max[S(\rho_{\text{A}}), S(\rho_{\text{B}})] - S(\rho_{\text{AB}}), \tag{14}$$

which for pure states coincides with entanglement of formation (or any other sensible choice of entanglement measure that all reduce to the marginal entropy in case of pure states). In the above equation it is assumed that bits which are sent down the communication channel are treated as classical in the sense that they are only dephased once, and not again in a second basis. This interplay led to subsequent investigations into the thermodynamic nature of entanglement in [153], where analogies between irreversible operations in thermodynamics and bound entanglement were drawn, and to concrete physical scenarios satisfying this bound in [120].

4.4. Entanglement resources in thermodynamic tasks

Apart from resource theory inspired questions, one might study the role of informational quantities through their inevitable appearance in thermodynamic operations at the quantum level. For instance the role of entangling operations and entanglement generation in extracting

work from multiple copies of passive states , i.e. states where no local work extraction is possible [107, 108], has attracted some attention recently. The implied fact that global unitary operations are required to extract work indicates some form of non-local resource being involved in the process.

In general passive states are always diagonal in the energy eigenbasis [107, 108], which implies that one starts and ends the protocols with diagonal states. In these scenarios the individual batteries from which work is to be extracted are considered non-interacting, directly implying the separability of initial and final states in these protocols. Nonetheless the fact that local unitaries can never extract any work from copies of passive states directly implies that entangling unitaries enable work extraction from such states [154]. In that sense entangling power of unitaries can be seen as a resource for work extraction purposes (which in conventional thermodynamic resource is of course considered a free operation).

In [155] the role of quantum resources in this context was further explored. While it is true that the ability to perform entangling unitaries is required for this particular work extraction problem, this does not imply that any entanglement is ever generated in the process. In fact the whole procedure can dynamically be implemented without ever generating the slightest bit of entanglement [155], however the most direct transformation can considerably entangle the systems in the process. In [156] it was demonstrated that if the work per unit time (power) is considered with cyclic operations in mind then a quantum advantage for charging power can be achieved.

4.5. Using thermodynamics to reveal quantumness

That entanglement plays a special role in quantum many-body physics is a well established fact that has received adequate attention in numerous publications (see e.g. [157] and the extensive list of citations therein). In this topical review we want to at least mention a related question that connects quantum thermodynamics directly with entanglement theory: the possibility to use thermodynamic observables to reveal an underlying entanglement present in the system. At zero temperature it is already known that many natural interaction Hamiltonians have entangled ground states (in fact often many low energy eigenstates even of local Hamiltonians feature entanglement). This fact can be exploited to directly use the energy of a system as an entanglement witness, even at non-zero temperatures [158]. Intuitively this can be understood through the fact that a low average energy directly implies that the density matrix is close to the entangled ground state. If this distance is sufficiently small that can directly imply entanglement of the density matrix itself. The known results and open questions of this interplay including [159–166] are also discussed in the review [36]. Furthermore, other macroscopic thermodynamic quantities can also serve as entanglement witnesses through a similar intuition, such as e.g. the magnetic susceptibility [167] or the entropy [168].

4.6. Outlook

Resource theories always have their foundation in what we believe to be hard/impossible to implement and what resources allow us to overcome such limitations. As such they always only capture one specific aspect of the physical systems under investigation. The results outlined in this section emphasize the fact that thermodynamic constraints have drastic consequences for processing quantum information and that locality constraints will change thermodynamic considerations at the quantum scale. One path to explore could now be a consistent resource theory that adaptively quantifies possible resources from different

restrictions. This would furthermore elucidate the exact role played by genuine quantum effects, such as entanglement, in thermodynamics.

5. Quantum fluctuation relations and quantum information

5.1. Introduction

The phenomenological theory of thermodynamics successfully describes the equilibrium properties of macroscopic systems ranging from refrigerators to black holes that is the domain of the large and many. By extrapolating backwards, from the domain of the 'many' to the 'few', we venture further from equilibrium into a regime where both thermal and quantum fluctuations begin to dominate and correlations proliferate. One may then ask the question— what is an appropriate way to describe this blurry world which is dominated by deviations from the average behaviour?

   One way to describe the thermodynamics of small systems where fluctuations cannot be ignored is by using the framework of stochastic thermodynamics [169]. In this approach the basic objects of traditional statistical mechanics such as work and heat are treated as stochastic random variables and hence characterized by probability distributions. Over the last 20 years various approaches have lead to sets of theorems and laws, beyond the linear response regime, which have revitalized the already mature study of non-equilibrium statistical mechanics. Central to these efforts are the fluctuation relations that connect the non-equilibrium response of a system to its equilibrium properties. A wealth of results have been uncovered in both the classical and the quantum regimes and the interested reader is directed to the excellent reviews on the topics [21–23]. Here we focus on aspects of this approach that have been specifically influenced by concepts in quantum information, or show promise for symbiosis. We hope that by reviewing the existing contributions as well as suggesting possible research avenues, further cross fertilization of the fields will occur.

   To begin with, it is useful to illustrate how the probability distributions of a thermodynamic variable like work is defined. Consider a quantum system with a time-dependent Hamiltonian $H(\lambda(t))$, parametrized by the externally controlled *work parameter* $\lambda(t)$. The system is prepared in a thermal state by allowing it to equilibrate with a heat bath at inverse temperature β for a fixed value of the work parameter $\lambda(t < t_{\rm i}) = \lambda_{\rm i}$. The initial state of the system is therefore the Gibbs state

$$\tau(\lambda,\,\beta) := \frac{{\rm e}^{-\beta H(\lambda_{\rm i})}}{\mathcal{Z}_{\beta}(\lambda_{\rm i})}.$$

At $t = t_{\rm i}$ the system-reservoir coupling is removed and a fixed, reversible protocol is performed on the system taking the work parameter from its initial value $\lambda_{\rm i}$ to the final value $\lambda_{\rm f}$ at a later time $t = t_{\rm f}$. The initial and final Hamiltonians are defined by their spectral decompositions

$$H(\lambda_{\rm i}) = \sum_{n} E_n(\lambda_{\rm i})\, |\psi_n\rangle\langle\psi_n|$$
$$\text{and}\quad H(\lambda_{\rm f}) = \sum_{m} E_m(\lambda_{\rm f})\, |\phi_m\rangle\langle\phi_m|$$

respectively, where $|\psi_n\rangle$ ($|\phi_m\rangle$) is the nth (mth) eigenstate of the initial (final) Hamiltonian with eigenvalue $E_n(\lambda_{\rm i})$, $E_m(\lambda_{\rm f})$. The protocol connecting the initial and final Hamiltonians generates the unitary evolution operator $U(t_{\rm f}, t_{\rm i})$, which in general has the form

$$U(t, t_{\mathrm{i}}) = \mathbf{T}_{\rightarrow} \exp\left[-\mathrm{i} \int_{t_{\mathrm{i}}}^{t} \mathrm{d}t' \, H(\lambda(t')) \right], \tag{15}$$

where $\mathbf{T}_{\rightarrow}$ denotes the time-ordering operation. We stress here that, in this framework, one typically assumes that the system is initially prepared in a thermal state but after the unitary protocol the system is generally in a non-equilibrium state.

The work performed (or extracted) on (or from) the system as a consequence of the protocol is defined by the outcomes of two projective energy measurements [170]. The first, at $t = t_{\mathrm{i}}$, projects onto the eigenbasis of the initial Hamiltonian $H(\lambda_{\mathrm{i}})$, with the system in thermal equilibrium. The system then evolves under the unitary operator $U(t_{\mathrm{f}}, t_{\mathrm{i}})$ before a second projective measurement is made onto the eigenbasis of the final Hamiltonian $H(\lambda_{\mathrm{f}})$ at $t = t_{\mathrm{f}}$. The joint probability of obtaining the outcome $E_n(\lambda_{\mathrm{i}})$ for the initial measurement followed by $E_m(\lambda_{\mathrm{f}})$ for the final one is easily shown to be

$$p(n, m) = \frac{\mathrm{e}^{-\beta E_n(\lambda_{\mathrm{i}})}}{\mathcal{Z}(\lambda_{\mathrm{i}})} \, |\langle \phi_m | \, U(t_{\mathrm{f}}, t_{\mathrm{i}}) | \psi_n \rangle|^2. \tag{16}$$

Accordingly, the quantum work distribution is defined as

$$P_{\mathrm{F}}(W) = \sum_{n,m} p(n, m) \, \delta(W - [E_m(\lambda_{\mathrm{f}}) - E_n(\lambda_{\mathrm{i}})]), \tag{17}$$

where δ is the Dirac delta function. For reasons which will become clear shortly we use the subscript F to denote 'forward' protocol. Physically, equation (17) states that the work distribution consists of the discrete number of allowed values for the work $(E_m(\lambda_{\mathrm{f}}) - E_n(\lambda_{\mathrm{i}}))$ weighted by the probability $p(n, m)$ of measuring that value in a given realization of the experiment. The quantum work distribution therefore encodes fluctuations in the measured work arising from thermal statistics (first measurement) and from quantum measurement statistics (second measurement).

In order to understand what is meant by a fluctuation theorem, we introduce a backward process which is the time reversed protocol of the forward one previously defined. Now $P_{\mathrm{B}}(W)$ is the work distribution corresponding to the *backward process*, in which the system is prepared in the Gibbs state of the final Hamiltonian $H(\lambda_{\mathrm{f}})$ at $t = 0$ and subjected to the time-reversed protocol that generates the evolution $\Theta U(t_{\mathrm{f}}, t_{\mathrm{i}}) \Theta^{\dagger}$, where Θ is the anti-unitary time-reversal operator. It turns out that the following theorem holds, the Tasaki–Crooks relation [171, 172],

$$\frac{P_{\mathrm{F}}(W)}{P_{\mathrm{B}}(-W)} = \mathrm{e}^{\beta(W - \Delta F)}, \tag{18}$$

which shows that, for any closed quantum system undergoing an arbitrary non-equilibrium transformation, the fluctuations in work are related to the equilibrium free energy difference for the corresponding isothermal process between the equilibrium states $\tau(\lambda_{\mathrm{i}})$ and $\tau(\lambda_{\mathrm{f}})$,

$$\Delta F = \frac{1}{\beta} \ln\left(\frac{\mathcal{Z}_{\beta}(\lambda_{\mathrm{i}})}{\mathcal{Z}_{\beta}(\lambda_{\mathrm{f}})} \right). \tag{19}$$

This relationship is further emphasized by a corollary to equation (18) known as the Jarzynski equality [173],

$$\int \mathrm{d}W P_{\mathrm{F}}(W) \mathrm{e}^{-\beta W} = \langle \mathrm{e}^{-\beta W} \rangle = \mathrm{e}^{-\beta \Delta F} \tag{20}$$

which states that ΔF (of the corresponding isothermal process) can be extracted from by measuring the exponentiated work. A straightforward application of Jensen's inequality for

convex functions allows one the retrieve the expected expression $\langle W \rangle \geqslant \Delta F$. The average energetic deviation of a non-equilibrium process from the equivalent reversible isothermal process is known as dissipated work

$$\langle W \rangle_{\mathrm{diss}} = \langle W \rangle - \Delta F. \tag{21}$$

Due to the Jarzynski equality this quantity is positive, $\langle W \rangle_{\mathrm{diss}} \geqslant 0$. This can be also directly seen from the Crooks relation, taking the logarithm of both sides of the equality in equation (18) and integrating over the forward distribution we find

$$\langle \Sigma \rangle = \beta(\langle W \rangle - \Delta F) = K(P_{\mathrm{F}}(W) \| P_{\mathrm{B}}(-W)), \tag{22}$$

where K is the classical Kullback Leibler divergence and we have introduced the average irreversible entropy change $\langle \Sigma \rangle$ corresponding to the dissipated work. Physically the irreversible entropy change, in this context, would be the internal entropy generated due to the non-equilibrium process which would manifest itself as an additional source of heat if an ideal thermal bath would be reconnected to the system at the end of the protocol. In [174] it was shown that the irreversible entropy change can also be expressed in terms of a quantum relative entropy

$$\langle \Sigma \rangle = D(\sigma \| \tau(\lambda_{\mathrm{f}}, \beta)) \tag{23}$$

where $\sigma = U(t_{\mathrm{f}}, t_{\mathrm{i}}) \tau(\lambda_{\mathrm{i}}, \beta) U^{\dagger}(t_{\mathrm{f}}, t_{\mathrm{i}})$ is the out of equilibrium state at the end of the protocol. This is fully consistent with the open system treatment in [175].

5.2. Phase estimation schemes for extraction of quantum work and heat statistics

Surprisingly, the proposals to measure the characteristic perhaps one of the most important contributions that ideas from quantum information have made to this field in statistical mechanics is the experimental acquisition of statistics of work. In the classical setting considerable progress has been made in the experimental extraction of the relevant stochastic thermodynamic distributions to explore and verify the fluctuation theorems [23]. Up until very recently, no such experimental progress had been made for quantum systems. A central issue is the problem of building the quantum work distribution as it requires to make reliable projective energy measurements on to the instantaneous energy eigenbasis of an evolving quantum system [22, 170]. It was proposed in [176] that these measurements could be reliably performed on a single trapped ion, an experiment that was recently performed [177].

Alternatives to the projective method have been proposed [178, 179], based on *phase estimation schemes*, well known in quantum information and quantum optics [180]. In these schemes, we couple our system to an ancillary system, and perform tomography on that system. The spirit is very similar to the DQC1 algorithm put forward in [181]. The characteristic function of the work probability distribution (equation 24) can be obtained from the ancilla, and the work statistics are then extracted by Fourier transform. The *characteristic function* is defined as

$$\chi_{\mathrm{F}}(u) = \int \mathrm{d}W \, \mathrm{e}^{\mathrm{i}uW} P_{\mathrm{F}}(W). \tag{24}$$

The proposals to measure the characteristic function were first tested in the laboratory only quite recently in a liquid state NMR setup [182]. This experiment is the first demonstration of the work fluctuation theorems and extraction of work quantum statistics, and is expected to inspire a new generation of experiments at the quantum level. Another interesting extension of these schemes is to go beyond the closed system paradigm and to study open system dynamics at and beyond the weak coupling limit. The first extensions have been proposed in

[183–185]. In [186] the proposal outlined in [185] to measure the statistics of dissipated heat was implemented in order to perform a study of the information to energy conversion in basic quantum logic gates at the fundamental Landauer Limit.

Another interesting suggestion made to access the quantum work statistics is the use the concept of a 'positive operator valued measure', or POVM [187], a well-known concept within quantum information and quantum optics. A POVM is the most general way to describe a measurement in a quantum system, with the advantage that it can always be seen as a projective measurement on an enlarged system. In this work the authors show that by introducing an appropriate ancilla that the POVM description allows the work distribution to be efficiently sampled with just a single measurement in time. In this work it was suggested that the algorithm proposed could be used, in combination with the fluctuation theorems, to estimate the free energy of quantum states on a quantum computer. The scheme was recently extended and developed in [188] along with a promising implementation using ultra-cold atoms. This would be a promising avenue to explore work statistics in a many-body physics setting where the statistics of work can be shown to have universal behaviour at critical points [189].

5.3. Fluctuation relations with feedback, measurement and CPTP maps

The relationship between thermodynamics and the information processing is almost as old as thermodynamics itself and is no where more dramatically manifested than by Maxwell's demon [2–6]. One way of understanding the demon paradox is by viewing the demon as performing feedback control on the thermodynamic system. In this case the framework for stochastic thermodynamics and the fluctuation theorems needs to be expanded. Building upon previous work [151, 152], Sagawa and Ueda have generalized the Jarzynski equality to incorporate the feedback mechanism [190, 191] for classical systems. This theoretical breakthrough allowed for an experimental demonstration of information to energy conversion in a system by means of of non-equilibrium feedback of a Brownian particle [192]. These feedback based fluctuation theorems were further modified to incorporate both initial and final correlations [193]. These works, in particular, highlight the pivotal role played by mutual information in non-equilibrium thermodynamics [6].

The Sagawa–Ueda relations were generalized to quantum systems in [194]. For reasons of pedagogy we will follow this approach here. In the work of Morikuni and Tasaki an isolated quantum system is considered where an external agent has control of the Hamiltonian parameters. The system is initialized in a canonical state, $\tau(\beta)$, and an initial projective measurement of the energy is made whose outcome is E_i^0. The Hamiltonian is then changed via a fixed protocol and evolves according to the unitary operator U. In the next stage a projective measurement is performed with outcomes $j = 1,...,n$ and described by a set of projection operators $\Pi_1,...,\Pi_n$. Now the time evolution is conditioned on the outcome j so the Hamiltonian is changed according to these outcomes. This is the feedback control stage. Finally, one makes a projective measurement of the energy of the final Hamiltonian with outcome E_k^j. In this setting it is shown that

$$\langle e^{\beta(W-\Delta F)} \rangle = \gamma, \tag{25}$$

where $W = W_{i,j,k} = E_i^0 - E_k^j$ is the work and ΔF is the free energy difference between the initial state and the canonical state corresponding to the final value of the Hamiltonian H^j. We see that in this feedback controlled scenario a new term enters on the right hand side. A straightforward calculation shows that this term evaluates as $\gamma = \sum_j \text{tr}[\Pi_j U_j^\dagger \tau(\beta) U_j \Pi_j]$. This γ quantity is shown in [190, 194] to be related to the efficiency of the demon in making use of

the information it acquires during the feedback process. When it becomes less than one it provides an example of a failed demon who did not make a good use of the information acquired. On the other hand it can become larger than one indicating that the feedback is working efficiently. Another relation discovered by Sagawa and Ueda and quantized by Morkikuni and Taskaki concerns almost the same protocol as just explained only now classical errors are made in the intermediate measurement stage. Again let the intermediate measurement be described by $\Pi_1, \ldots, \Pi_n$ which yield the result j but the controller misinterprets the result as j' with a certain probability. In this framework another generalized fluctuation theorem can be derived

$$\langle e^{\beta(W - \Delta F - I)} \rangle = 1, \tag{26}$$

where I is the mutual information between the set of measurement outcomes the demon actually records and what is the true result of the projection. These feedback fluctuation theorems for quantum systems were further generalized to the situation when a memory system is explicitly accounted for in [144] and shed light on the amount of thermodynamic work which can be gained from entanglement. In addition to feedback, fluctuation theorems were investigated under continuous monitoring [195, 196] and analysed for general measurements [197, 198].

A recent series of papers have analysed fluctuation-like relations from the operational viewpoint employing the full machinery of trace-preserving completely positive maps. In [199] the formalism is used to give an alternative derivation of the Holevo bound [200]. In [201] an information-theoretical Jarzynski equality was derived. It was found that fluctuation relations can be derived if the map generated by the open dynamics obeys the unital condition. This has been connected to the breakdown of micro-reversibility for non-unital quantum channels [202–205]. In [206] the authors analysed the statistics of heat dissipated in a general protocol and found that the approach can be used to derive a lower bound on the heat dissipated for non-unital channels. Recently this bound has been used to investigate the connection with the build up of multipartite correlations in collisional models [207].

5.4. Entropy production, relative entropy and correlations

With the surge of interest in the thermodynamics of quantum systems and the development of quantum fluctuation relations, research has been directed to microscopic expressions for entropy production. In formulating thermodynamics for non-equilibrium quantum systems, the relative entropy plays a central role [191]. As first pointed out in [208] this is due to its close relationship with the free energy of a quantum state. The relative entropy also plays a central role in quantum information theory, in particular, in the geometric picture of entanglement and general quantum and classical correlations [209, 210]. In the non-equilibrium formulation of thermodynamics [22] it is omnipresent for the description of irreversible entropy production in both closed [174] and open driven quantum systems [211] (see also [212]). One may then wonder if there exists a relationship between the entropy produced by operations that generate or delete correlations in a quantum state and the measures for correlations in that state? Given the youthful nature of the field the question is largely unanswered but some progress in this direction has been made.

The relationship between the relative entropy of entanglement and the dissipated work was first proposed as an entanglement witness in [213]. Going beyond the geometric approach a functional relationship between the entanglement generated in a chain of oscillators and the work dissipated was explored in [214] and also later for more general quantum correlations [215]. In an open systems framework it was shown that the irreversible entropy production

maybe attributed to the total correlations between the system and the reservoir [216] (we note that this derivation is entirely analogous to the formulation of the Landauer principle put forward by in [115]). The exchange fluctuation relation and the consequences for correlated quantum systems were studied in [217].

5.5. Outlook

As fluctuation theorems are exact results, valid for arbitrary non-equilibrium dynamics, they are currently being used to understand the nonlinear transport of energy, heat and even information in quantum technologies. This is a relatively new research avenue and the applications of quantum fluctuation theorems in other fields such as condensed matter physics, quantum optics and quantum information theory are in their infancy. Ultimately, the hope would be that they provide a unifying framework to understand the relationship between information and energy in non-equilibrium quantum systems. Ultimately one would like to form a picture of information thermodynamics of quantum systems under general non-equilibrium conditions.

As we have seen above, quantum phase estimation, a central protocol in quantum information theory, has been applied successfully to extract work statistics from a small non-equilibrium quantum system and perhaps other such unexpected interdisciplinary links will emerge. For example one wonders if existing experimental schemes could be modified to deal with situations dealing with non-passive initial states so as to study maximal work extraction problems and also to extend to more complicated many-body and open system scenarios.

In [119, 218, 219] the first steps towards unification of the work statistics and fluctuation theorems approach to thermodynamics and the single shot statistical mechanics approaches mentioned have been taken (see section 4). We are confident that other links will emerge between various approaches in the not so distant future.

6. Quantum thermal machines

In this final brief section of the review we end by considering the area of quantum thermodynamics concerning quantum thermal machines, that is quantum versions of heat engines or refrigerators. We shall overview the extent to which quantum entanglement and correlations are relevant to their operation.

Whereas in almost all of the above the situation comprised of only one thermal bath and systems in contact with it, in this section our interest is in situations involving two (or more) thermal baths. Now, there are two regimes which one can focus on: the primary one is usually the cyclic behaviour of systems interacting with the baths, or alternatively the steady state behaviour that is characterized by the currents of heat or work that can be maintained in the long time limit. The second regime is the transient one, and how the system reaches stationarity.

One way to think of the present situation is that the second thermal bath is the system out of equilibrium with respect to the first bath, and the goal is to produce resources (work, or a steady state current out of a cold bath) at optimal rates. From this perspective, the quantum machine plays the role of the 'bridge' or the 'mediator' which facilitates the operation of the larger thermal machine.

The history of quantum thermal machines is a long one, going back to the sixties with the invention of the maser, which can be seen as a heat engine [220], and received much attention over the following decades. A complete overview of the literature in this direction is far beyond the scope of the present review; however excellent recent overviews can be found in

[31–33]. In the present context, one important message from this body of work is that thermal machines comprised of as little as a single qutrit (3 level system), or of 2 or 3 qubits, can be constructed, that moreover can approach Carnot efficiency (the maximal possible efficiency of any machine). It is thus plausible that they may ultimately become important from the perspective of nanotechnology and implementations of quantum information processing devices. As such a full understanding of their quantum behaviour, including the correlations they can build up, is important. Here we review specifically those studies concerned with the role of entanglement and quantum coherence in the functioning of such small quantum thermal machines, both at the level of the machine, as well as in the bath, if pre-processing operations are allowed. We also look at the role of coherence in the transient behaviour when the refrigerator is first switched on. We review a recent proposal for a witness that quantum machines are provably outperforming their classical counterparts. Finally, we look at the idea of using thermal machines as a means of entanglement generation (switching the focus away from the traditions resources of work or heat currents).

A related idea is that of *algorithmic cooling*, which we summarize in example 5, and which was recently reviewed in [221].

6.1. Absorption refrigerators

The first machine we shall look at is a quantum model of an absorption refrigerator, a refrigerator which is not run by a supply of external work (which is the situation most customarily considered), but rather run by a source of heat. An absorption refrigerator is thus a device connected to three thermal reservoirs; a 'cold' reservoir at temperature β_C from which heat will be extracted; a 'hot' reservoir at inverse temperature β_H, which provides the supply of energy into the machine; and finally a 'room temperature' reservoir at temperature β_R into which heat (and entropy) will be discarded. The goal is to cool down the cold reservoir (i.e. extract heat from it).

There are a number of different figures of merit that one can consider to quantify the performance of the machine. The most commonly considered is the *coefficient of performance* $COP = Q_C/Q_H$, where Q_C and Q_H are respectively the heat currents flowing out of the cold the hot reservoirs (the COP is the analogous quantity to the efficiency for an absorption refrigerator; since the COP can be larger than 1 it cannot be thought of directly as an efficiency). The famous result of Carnot [222], a statement of the second law of thermodynamics, is that the efficiency (or COP) of all thermal machines is bounded as a function of the reservoir temperatures. In particular, for the specific case of an absorption refrigerator we have $COP \leqslant (\beta_R - \beta_H)/(\beta_C - \beta_R)$. Other relevant figures of merit are the power Q_C (i.e. neglecting how efficient the process is), the COP when running at maximal power, and the minimal attainable stationary temperature β_C^{st} for a cold object in contact with the bath.

Below we give a brief outline of the model under consideration, full details of which can be found in [223, 224]. Consider three qubits, each one in thermal contact with one of the three thermal baths, with local Hamiltonians $H_i = E_i |1\rangle\langle 1|$, for $i = C, R, H$ chosen such that $E_R = E_C + E_H$ to ensure that the system has a degenerate subspace of energy E_R formed by the states $|010\rangle$ and $|101\rangle$ (where we use the order C–R–H for the three qubits). In this subspace the interaction Hamiltonian $H_{int} = g(|010\rangle\langle 101| + |101\rangle\langle 010|)$ is placed, which mediates the transfer of energy. A schematic representation of this fridge can be found in figure 5.

Example 5. Algorithmic cooling. Consider a collection of n qubits, all at inverse temperature β, with corresponding populations in the ground and excited states p and

Schematic diagram of a three qubit autonomous refrigerator (inside circle), coupled to three thermal reservoirs. The interaction Hamiltonian is represented by the green and orange arrows.
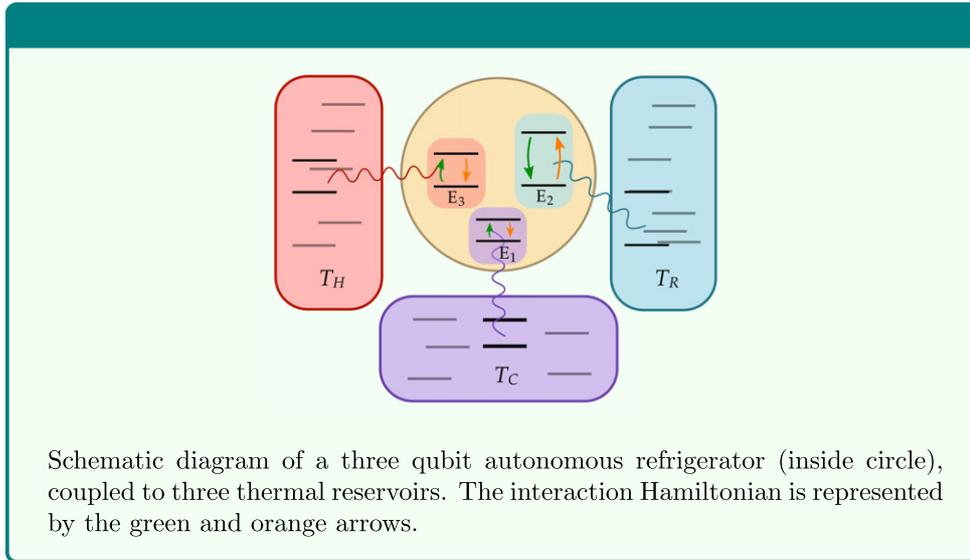
Figure 5. Three-qubit fridge.

$(1 - p)$ respectively. The goal of algorithmic cooling is to bring m qubits to the ground state by an arbitrary unitary transformation. A fundamental upper bound can be placed on m, purely by entropic considerations. The initial entropy is $nS(\tau(\beta) = nH(p)$, where $H(p) = -p \log_2 p - (1 - p) \log_2(1 - p)$ is the *binary Shannon entropy*. Since unitary transformations do not change the entropy, this easily leads to the upper bound on m,

$$m \leqslant n(1 - H(p)) \tag{27}$$

which would be achieved if the remaining $n - m$ qubits are all left at infinite temperature (maximally mixed state) with entropy $S(\tau(0)) = 1$. In [225] it was shown that as n tends to infinity this fundamental limit can be approached using an algorithm which uses $O(n \log_2 n)$ unitary gate operations. It was later realized that given access to an external bath this limit can be surpassed: the qubits which end this protocol at infinite temperature can be 'refreshed' to temperature β and the protocol can be run again on the remaining $(n - m)$ qubits, for example [226]. This is referred to as *heat-bath algorithmic cooling*.

In order to understand the basic principle, one can focus instead on three qubits and assume that the first is the one which is to be cooled down (now not to zero temperature, but any colder temperature). Let us consider the populations of the two states $|100\rangle$ and $|011\rangle$, which are $p^2(1 - p)$ and $p(1 - p)^2$ respectively. The state $|100\rangle$, in which qubit one is excited (and therefore 'hot') has more population than the state $|011\rangle$, where qubit one is in the ground state (and therefore 'cold'). Thus, by swapping the population of these two states the first qubit is cooled down. Indeed, after the application of such a unitary, the final population p' in the ground state of the first qubit is

$$p' = p + (2p - 1)p(1 - p) \tag{28}$$

which is greater than p whenever $(2p - 1) > 0$, i.e. whenever the first qubit was at a positive temperature. Finally, a unitary which implements $|011\rangle \leftrightarrow |100\rangle$ whilst leaving all other energy eigenstates the same can easily be constructed from the CNOT and Toffoli gates as
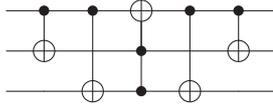
   A recent review giving many more details about algorithmic cooling can be found in [221].

6.1.1. Stationary behaviour.   Assuming the weak coupling regime between the qubits and the baths, the dynamics can be modelled using a time-independent Lindblad master equation $\dot{\rho} = \mathcal{L}(\rho)$ (with $\mathcal{L}$ the Linbladian, i.e. the most general generator of time-homogeneous, Markovian dynamics). The stationary solution ρ^{st}, satisfying $\mathcal{L}(\rho^{\mathrm{st}}) = 0$, can be shown to correspond to an absorption refrigerator if the parameters are chosen appropriately, i.e. such that $\beta_C^{\mathrm{st}} > \beta_C$, where β_C^{st} is the stationary inverse temperature of the cold qubit.

   From the point of view of quantum information, the basic questions about this steady state are (i) whether quantum correlations (for example entanglement) are present in the stationary state, and (ii) if yes, whether they are important for the operation, or merely a by-product of quantum evolution. These questions were addressed in [223, 224].

   In [224] quantum correlations in the form of discord were studied. The quantum discord $\mathcal{D}(AB)_\rho := I(A:B)_\rho - I(A:B)_\sigma$, with σ the state after a minimally disturbing measurement on Bob, is a form of quantum correlation weaker than entanglement [227, 228]. The authors studied quantum discord between numerous inequivalent partitions of the system. The most interesting results were obtained when the discord is calculated between the cold qubit (the qubit which is being cooled) and the relevant subspace of the two remaining qubits (that singled out by the interaction Hamiltonian H_{int}). They found that discord is always present, but they found no relationship between the *amount* of discord present and the rate at which heat was extracted from the cold bath. Specifically, to obtain this result they studied the behaviour of discord as a function of the energy spacing E_C of the cold qubit. Whilst both quantities typically exhibited local maxima as E_C was varied, these maxima failed to coincide.

   In [223] the focus was instead on the entanglement maintained in the steady state. First, if the machine is operating close to the maximal Carnot limit then the state is necessarily fully separable, i.e. a convex combination of product states of the three qubits. Conversely, operating far from this regime every type of multipartite entanglement can be found in the stationary state. In particular, there are regimes where entanglement is generated across any fixed bipartition, and even genuine multipartite entanglement can be found, demonstrating that the state has no biseparable decomposition. Here it must be stressed that the amount of entanglement found was small, but that this should be expected due to the weak inter-qubit coupling.

   Finally, it was also shown that there appears to be a link between the amount of entanglement generated in the partition R|CH and the so-called *cooling advantage* that entangled machines have compared to separable ones. In particular, the cooling advantage was defined as the difference between the minimal possible temperatures that could be achieved with either separable or entangled refrigerators. More precisely, by optimizing the stationary temperature β_C^{st} of the cold qubit, varying the Hamiltonian of the machine qubits and their couplings to the baths (at fixed temperatures). It was shown that arbitrary machines (i.e. ones allowed to be entangled) could outperform ones which were additionally constrained to be separable. Moreover, the advantage was found to be a function only of the amount of entanglement generated across the R|CH partition. One point of interest is that this is the bipartition of energy entering versus energy leaving the machine, thus suggesting a connection between the transport properties of the machine and the entanglement.

6.1.2. Transient behaviour. Instead of looking at the steady state behaviour, one may also consider the transient behaviour. Such questions are relevant when one is interested in running a small number of cooling cycles in order to cool down the system as fast as possible. Alternatively, if one is thinking of initializing a system for some other use, the transient regime might also be of interest for quicker initialization. Intuitively, since the evolution between the qubits is coherent, one might expect the local populations to undergo Rabi oscillations, and hence by running for precise times lower temperatures may be achievable in a transient regime (as the qubits continuous cool down and heat up).

This is precisely what was shown in [229, 230]. More precisely, in [230] the authors study the Markovian dynamics with weak inter-qubit coupling g (relative to the relaxation rates, as in the above subsection), while in [229] the authors considered additionally Markovian dynamics with strong inter-qubit coupling, and band-limited non-Markovian baths (modelled with a one-qubit memory for each machine qubit). Taking as the natural initial state the product state, whereby each qubit is initially at the same temperature as the bath, both numerically study the transient behaviour of the temperature of the cold qubit as the system approaches stationarity. While in the weak interaction case no Rabi oscillations are observed (since the system is effectively over-damped), in the strong-interaction case Rabi oscillations indeed take place, with period approximately $2\pi/g$. This demonstrates that coherent oscillations offer an advantage for cooling. A more complicated behaviour due to memory effects is also observed in the non-Markovian case in [229], but nevertheless the system can be seen to pass through much colder temperatures during its transient behaviour. In [230] it was also shown that if the couplings are chosen appropriately, (in particular such that the weakest coupling is to the hot reservoir), then the system remains for a long time at a temperature below the stationary temperature, in particular without oscillating above it. This demonstrates a particular stable regime for the preparation of the system at temperatures below its stationary temperature.

In order to explore more the advantage offered by coherence, [229] also considered varying the initial state, by altering the coherence in the subspace where the Hamiltonian operates. Interestingly, with only a small amount of initial coherence, even when considering case (a) of weak-interaction dynamics, oscillations in the temperature are seen, again allowing for cooling below the stationary temperature. In the other two cases, the magnitude of the oscillations is also seen to increase (i.e. the system achieves lower temperatures transiently), demonstrating an advantage in all situations.

Finally, in [230] the amount of entanglement that is generated in the transient regime was also studied. Focusing on either genuine multipartite entanglement, or entanglement across the partition R|CH, i.e. the one corresponding to energy-in versus energy out (as studied in [223]), considerably more entanglement can be generated in the transient regime.

6.2. Reservoir engineering

As we have seen in previous sections of the review, thermals states are naturally considered as a free resource which can be utilized and manipulated. Likewise, the ubiquity of thermal machines is that having access to two large thermal reservoirs can also be considered as something essentially free, and thermal machines consider ways of utilizing these resources.

One interesting avenue is to consider that any transformation of a thermal reservoir which can 'easily' be carried out can also be considered to be free, as an idealization, and this motivates the idea of considering thermal machines which run between *engineered reservoirs*, assuming that the engineering was an easy to perform transformation. In the present context, when one has sufficient control over (part of) the reservoir, then the engineering can be at the

quantum level. Here again we are interested specifically in the role that quantum correlations engineered in the bath have on the functioning of quantum thermal machines.

In [231, 232] reservoir engineering in the form of *squeezing* is considered, since squeezing is relatively easy to carry out, and is furthermore known to offer quantum advantages in other contexts in quantum information. That is the reservoir, instead of consisting of a large collection of modes in thermal states at inverse temperature β_H, are in fact squeezed thermal states (at the same temperature). More precisely, the squeezing operator is $U_{sq} = \exp((ra^2 - r*a^{\dagger 2})/2)$ with a and $a^{\dagger}$ the annihilation and creation operators respectively, and the squeezed thermal state (of a given mode, i.e. a harmonic oscillator) is $U_{sq}\tau(\beta)U_{sq}^{\dagger}$. Whereas normally the variances of the quadratures ($x = (a + a^{\dagger})/2$ and $p = (a - a^{\dagger})/2i$) are symmetric, the squeezed modes become asymmetric, with the former amplified by the factor e^r, and the latter shrunk by e^{-r}. The important point is that a system placed in thermal contact with such a squeezed reservoir will not thermalize towards a thermal state at β, but rather to a squeezed thermal state, which has the same average number of photons as a thermal state at temperature $\beta(r) < \beta$. That is, in terms of average number of photons, a squeezed thermal state appears 'hotter' than a thermal bath.

Starting first with [232], a model of an absorption refrigerators is considered, identical to the one outlined in the previous section. Here, in accordance with the above, in the weak coupling regime the effect of the reservoir engineering amounts to modifying the Linbladian $\mathcal{L}$, such that the term corresponding to the hot reservoir $\mathcal{L}_H$ transforms to $\mathcal{L}_H(r)$, where this now generates dissipation towards the squeezed thermal state at $\beta_H(r)$. They show that the maximal COP that the refrigerator can approach becomes

$$\eta(r) = \frac{\beta_R - \beta_H(r)}{\beta_C - \beta_R} > \eta_c = \frac{\beta_R - \beta_H}{\beta_C - \beta_R}. \tag{29}$$

That is, the COP overcomes the Carnot limit that bounds the COP of any absorption refrigerator operating between baths at β_C, β_R and β_H, if reservoir engineering is not carried out. Thus if reservoir engineering is more readily available than a hotter 'hot' bath, then this approach clearly provides an advantage in terms of the COP.

In [231] a different model was considered, this time a quantum heat engine operating a quantum Otto cycle, a time dependent cycle, comprising two expansion stages (changing the Hamiltonian of the system) and two thermalization stages. The system considered comprised of a single harmonic oscillator, with initial spacing E_1. While uncoupled to any environment, the first stage is an expansion, whereby $E_1 \rightarrow E_2 > E_1$, i.e. the Hamiltonian is changed in time. In the second stage the system is then placed in contact with a squeezed hot reservoir (this is the stage which differs from a standard Otto cycle, where an unsqueezed hot reservoir is used). After disconnection, the third stage is a compression stage, bringing the spacing back from E_2 to E_1. Finally, the system is placed in contact with a cold (unsqueezed) reservoir, in order to thermalize at the cold temperature. This cycle is summarized in figure 6. The authors perform an analysis of the system and similarly show that the maximum efficiency of the engine exceeds the Carnot efficiency (of the Otto cycle, $\eta = \beta_H/\beta_C$). Moreover, if one considers the efficiency at maximum power, then this can also be surpassed, and as the squeezing parameter becomes large, the efficiency at maximum power approaches unity.

Finally, we stress that these results do not constitute a violation of the second law, since they consider a scenario outside the regime of applicability of the Carnot limit (much in the same way that a regular car engine, consuming fuel, does not violate the second law, since it is also outside the regime of applicability). Conversely, it is interesting that the net effect of squeezing appears to be *as if* the hot reservoir has been heated to a temperature $\beta_H(r)$, and
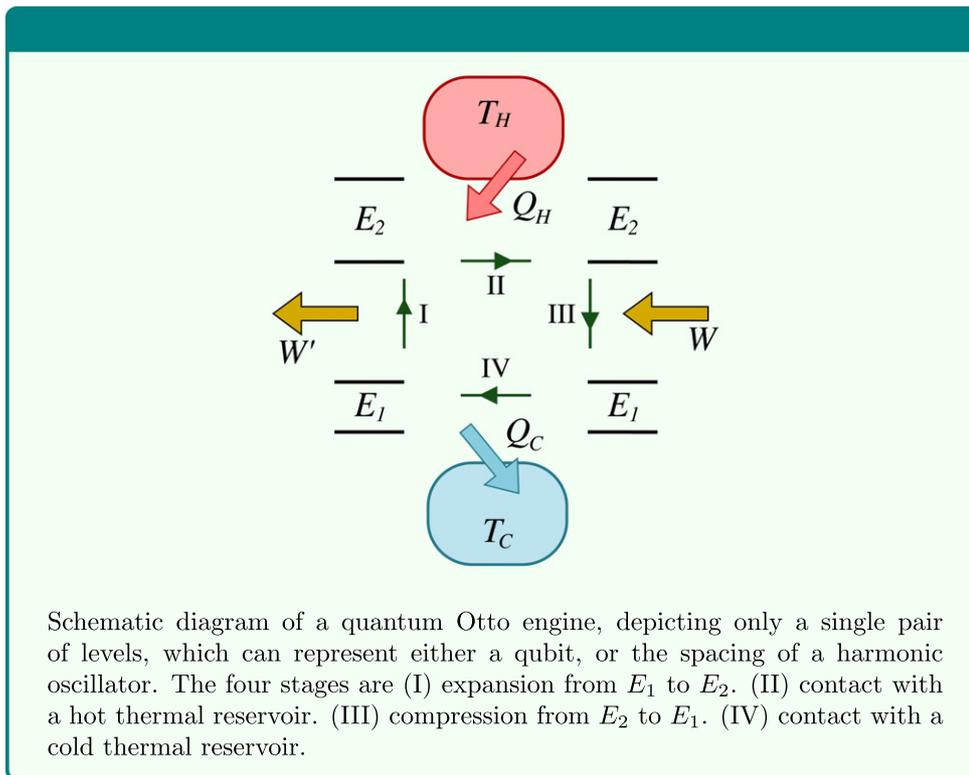
Schematic diagram of a quantum Otto engine, depicting only a single pair of levels, which can represent either a qubit, or the spacing of a harmonic oscillator. The four stages are (I) expansion from E_1 to E_2. (II) contact with a hot thermal reservoir. (III) compression from E_2 to E_1. (IV) contact with a cold thermal reservoir.

Figure 6. Quantum Otto engine.

that the performance of the machines is bounded exactly by the Carnot limit with respect to this new temperature.

6.3. Quantum thermodynamic signatures

One way to differentiate between a system which is genuinely using quantum effects and one which is only using the formal structure of quantum mechanics (the discreteness of energy levels, for example) is to devise signatures, or witnesses, for quantum behaviour. This is similar to what is done in entanglement theory, or in Bell nonlocality, where one finds witnesses which certify that entanglement was present, since no separable quantum state could pass a certain test. An interesting question is whether one can find analogous witnesses in a quantum thermodynamics setting. This is what was proposed in [233] in the form of *Quantum thermodynamic signatures*.

In more detail, the main idea of [233] is to find a threshold on the power of a thermal machine which would be impossible to achieve for a machine which is 'classical'. The authors take as the minimal set of requirements for a machine to be considered classical (i) that it's operation can be fully described using population dynamics (i.e. as a rate equation among the populations in the energy eigenbasis); (ii) that the energy level structure and coupling strengths are unaltered compared to quantum model under comparison; (iii) that no new sources of heat or work are introduced. A way to satisfy the above three constraints is to add pure de-phasing noise in the energy eigenbasis on top of the dissipative dynamics of the

quantum model (arising from the interaction with the thermal reservoirs). One can then compare models with and without de-phasing noise, and ask whether the additional noise places an upper bound on the power of the machine.

For simplicity in presentation, in what follows we will focus here on the results obtained for the four-stage qubit Otto heat engine, similar to the one described in the previous subsection (except now with a qubit in place of a harmonic oscillator). We note that the authors show that the same results hold for a two-stage engine [234] and for continuous time engines [25], as well as for refrigerators and heat pumps. As an aside, the reason why the result holds for all three models is because [233] also proves that in the regime of weak-coupling to the bath, and weak driving, all three types of engine can be shown to be formally equivalent, producing the same transient and steady state behaviour at the level of individual cycles.

It is shown that a state independent bound can be placed on the power of a classical machine which is proportional to the duration of a single cycle of the engine τ_{cyc}, as long as the so-called 'engine-action' s is small, where the engine action is the product of the duration τ and energy scale (as measured by the operator norm of each term appearing in the Master equation). They demonstrate that there is a regime where a quantum engine (i.e. one without additional dephasing) can provably outperform the corresponding classical machine, with powers an order of magnitude larger in the former case.

6.4. Stationary entanglement

Entanglement is understood to be a fragile property of quantum states, that is one typically expects that noise will destroy the entanglement in a quantum state. Much effort has been invested in investigating and devising ways in which one can counter the effects of noise, and maintain entanglement in a system, such as quantum error correction, dynamical decoupling, decoherence free subspaces, to name but a few.

In the first subsection we saw that the non-equilibrium steady state of autonomous quantum thermal machines can be entangled. If one thus focuses not on their thermodynamic functioning, but rather on their entanglement functioning, we see that whenever a thermal machine reaches a steady state which is entangled, this constitutes a way of generating stead state entanglement, merely through dissipative interactions with a number of thermal environments at differing temperatures.

Furthermore, if the interest is only in steady state entanglement generation, then it is not even necessary that the machine perform any standard thermodynamic task, and can in fact simply be a *bridge* between two reservoirs, allowing the steady flow of heat from hot to cold such that the stationary state of the bridge is necessarily entangled. This is precisely the situation which was first considered in [235], where the minimal system of two qubits interacting with two baths at temperatures β_{H} and β_{C} was considered in the weak coupling (Markovian) regime. Numerous variants were then discussed: in [236–240] different aspects of the dynamical approach to the steady state were analysed (assuming non-Markovian dynamics, the rotating wave approximation, etc); in [241, 242] a 3 qubit bridge was considered; in [243] the stationary discord was also studied; in [244, 245] geometric and dielectric properties of the environment were considered, and in [246] superconducting flux qubits and semiconductor double quantum dot implementations were explored.

Focusing on the simplest possible example, that of the two qubit bridge, the take home message of this line of investigation is that this is a viable means to generate stationary entanglement. In particular the implementations considered in [246] suggest that in experimentally accessible situations steady state entanglement can indeed be maintained at a level which might be usable to then later distill.

6.5. Outlook

We have seen in this section a range of results concerning quantum thermal machines, focusing primarily on the quantum correlations and entanglement present in the machine, as well as other signatures of quantumness. Although we have focused on the progress that has been achieved so far, there are a number of directions which should be explored in further work to more fully understand the role of quantum information for quantum thermal machines.

First of all, the main playground of study in this section has been the weak-coupling regime, where the machine is in weak thermal contact with the thermal reservoirs. It is important and interesting to ask what happens outside of this regime, when the thermal baths are strongly coupled to the machine. On the one hand, intuition suggests that stronger coupling corresponds to more noise, which will be detrimental to fragile quantum correlations. On the other hand, stronger driving might lead to more pronounced effects. As such, the interplay between noise and driving needs to be better understood.

Second, we have seen that quantum signatures, either in terms of entanglement or coherence, can be constructed, which show that there is more to quantum thermal machines than just the discreteness of the energy levels. Here, it would be advantageous to have more examples of quantum signatures, applicable in as wide a range of scenarios as possible. An experimental demonstration of a quantum signature would also be a great development concerning the implementation of thermal machines.

Finally, thinking of cooling as a form of error correction, it is interesting to know if ideas from quantum thermal machines can be incorporated directly into quantum technologies as a way to fight decoherence. This would be as an alternative to standard quantum error correction ideas, and an understanding of how they fit alongside each other could be beneficial from both perspectives.

7. Final remarks

Ideas coming from quantum information theory have helped us understand questions, both fundamental and applied, about the thermodynamic behaviour of systems operating at and below the verge at which quantum effects begin to proliferate. In this review we have given an overview of these insights. We have seen that they have been both in the form of technical contributions, for example with new mathematical tools for old problems, such as the equilibration problem, and also in the form of conceptual contributions, like the resource theory approach to quantum thermodynamics.

Although quantum information is only one of the many fields currently contributing to quantum thermodynamics, we expect its role to become more important as the field grows and matures. Indeed, we believe that placing information as a central concept, just as Maxwell did when his demon was born, will lead to a deeper understanding of many active areas of physics research beyond quantum thermodynamics.

Author contributions

All authors contributed equally to this review. Sections I and III were adapted from LdR's PhD Thesis [127].

Acknowledgments

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