### Quantum Demons

The name *Statistical Mechanics* actually came from the American physicist Josiah Willard Gibbs (1839-1903) in 1874. Inspired by the work of Maxwell and Boltzmann, he realized that this was an entirely new discipline and Gibbs developed his own system of statistical mechanics and defined an entropy in terms of ensembles [396]. He considered three types of ensembles: the micro canonical for systems that have definite energy, the canonical for systems in contact with heat baths and thus have fluctuating energies, and the grand canonical that has fluctuations in both energy and particle number. Bohr admired the ensemble approach of Gibbs and had said to Heisenberg "You read Gibbs and there are these chapters in Gibbs' book and that is really everything that can be said about thermodynamics." [398, p. 325] Gibbs' expression for the entropy in terms of states labeled by v takes the form:

$$S = -k \sum_{\nu} P_{\nu} \log P_{\nu}$$

where  $P_{\nu}$  is the probability of the microstate and  $\sum_{\nu} P_{\nu} = 1$ . Gibbs' expression for the entropy has the same form later found for quantum systems with discrete energy levels by von Neumann. The founders of quantum mechanics had worried about the issues of thermodynamic irreversibility and entropy change during measurement. As an example of one of many discussions, here from a 1947 letter from Bohr to Pauli and Pauli's response [398, p. 325].

Bohr to Pauli:

See the print edition of The Quantum Measurement Problem for quotation.

Pauli to Bohr:

See the print edition of The Quantum Measurement Problem for quotation.

The generalization of statistical mechanics to include quantum mechanics began with von Neumann in his 1927 paper, his 1929 paper on the quantum ergodic and H theorems, and his 1932 book, *Mathematical Foundations of Quantum Mechanics* [13]. Von Neumann had introduced his version of entropy based on considerations of the disorder of quantum states so that it has the same meaning as the thermodynamic entropy. The von Neumann entropy of the quantum density matrix  $\rho$  is

$$S(\rho) = -\mathrm{Tr}(\rho \log \rho)$$
.

For a system with discrete energy levels and using the eigenstates of the Hamiltonian to compute the trace, the von Neumann entropy takes the same form as the Gibbs entropy. Von Neumann had established a procedure to determine the equilibrium

distribution by requiring that the entropy becomes a maximum under certain subsidiary conditions. An important difference in quantum mechanics is the symmetries of the particles under permutations, which must be antisymmetric states for fermions or symmetric states for bosons. Von Neumann's 1929 paper "Proof of the ergodic theorem and the H-theorem in quantum mechanics," [584] revisited the problems of Boltzmann and Gibbs, and the issues of disorder and ergodicity, within the framework of quantum mechanics. As he summarizes in the introduction:

### See the print edition of The Quantum Measurement Problem for quotation.

Von Neumann's results have been newly revisited within the past decade with the renewed interest in quantum statistical mechanics [585]. Entropy production has been experimentally measured in a microscopic quantum system which breaks time-reversal invariance [586]. This utilized nuclear magnetic resonance of an ensemble of spin-1/2 particles from a Carbon-13 nucleus in a chloroform molecule in a liquid. The preparation in an initial thermal equilibrium state is what had singled out the preferred value of entropy, leading to irreversibility based on states that are most probable to occur, a microscopic quantum version of Boltzmann's arguments. Although ergodicity and time-averaging have often been used to justify entropy maximization in closed systems, ergodicity does not always appear to be applicable on the same regime over which statistical mechanics is successful in calculations [587]. This has generated recent attention in the fundamentals of quantum statistical mechanics [588], introducing the study of new concepts such as eigenstate thermalization of single quantum states, canonical typicality, and the relations between thermalization, integrability, and many-body localization. Can a closed quantum system actually behave as a thermal system? Thermalization of classical systems has been characterized in terms of concepts such as ergodicity and mixing, properties which enable systems to self-randomize. These properties reflect the statement that the most accessible microstates describe the same macroscopic state. However, the linear Schrödinger equation formally cannot exhibit such non-linear and chaotic behavior. A quantum many-body system initially in a pure state remains pure under unitary evolution with constant zero entropy. However, recent work has suggested that quantum systems can nevertheless thermalize, with indications that this is due to effectively thermal characteristics of the individual eigenstates so that expectation values are equal to their thermal values [587]. That this may happen for complex systems is called the *eigenstate thermalization hypothesis*. This was demonstrated experimentally using a Bose-Einstein condensate of Rubidium atoms in a twodimensional optical lattice in which the local entropy from quantum entanglement plays the role of a thermal entropy [589]. For a pure state of two spatially separated entangled spins, such as in a Bell state, the local measurement of one of the spins is a statistical mixture. If this indeed behaves as a thermalized state, it is expected to grow extensively with subsystem volume and the experiments are consistent with such an extensive thermal entropy.

The extension of Maxwell's demon to quantum systems has been studied

theoretically and experimental efforts on quantum demons have also begun with recent advances in techniques. However, Maxwell's demon exhibits new aspects quantum mechanically since measurement disturbs quantum states. More work can be extracted from a quantum demon than a classical demon [590] [591]. The indistinguishability of quantum particles affects the work that can be extracted [592]. Theoretical studies of Landauer's principle has been shown to apply in equilibrium quantum systems [593] [594] as well as non-equilibrium quantum systems [587]. The erasure of classical information encoded in quantum states by thermalization was considered by Lubkin [595]. For a system coupled to a thermal bath, the total entropy change on erasure of classical information encoded in quantum states by thermalization is the sum of the system and bath entropy changes with the minimum entropy change of the system given by [382]:

$$\Delta S_{svs} = k \ln 2S(\rho)$$

where  $S(\rho) = -\text{Tr}(\rho \log \rho)$  is the von Neumann entropy of the density operator  $\rho$ . The factor of *k* ln 2 is often customarily included for consistency with Landauer's principle. Landauer's principle has also been used to demonstrate the requirement of no-cloning for quantum states and the Holevo bound for accessible quantum information [596] [382].

Generalizing Maxwell's demon into the quantum realm has involved theoretical studies using quantum demons within classical engines [597] and also considering quantum demons within quantum engines [590], allowing a quantum treatment of the demon's entire cycle of operation including heat absorption, processing, decoherence, work generation and erasure. As an example, the energy stored in two-level systems can be utilized directly in scenarios where atoms are separated into different spatial paths and the energy is extracted from the atoms in the excited state and then recombining the paths. The which-way path information can then be erased isothermally and dissipated into the environment in preparation for the next cycle [598]. It has been suggested by Scully [599] [600] that quantum coherence of the ground state could be used to enhance the efficiency of the thermodynamic cycle beyond the Carnot efficiency by extracting work in the form of photons from a heat bath, quantum coherence playing the role of the demon in a quantum version of a Szilard one-molecule engine. Sorting occurs because cold atoms absorb less than they would otherwise in the absence of coherence whereas hot atoms emit photons. It has been proposed [601] that the information gained from measurements of the microlevels could also extract additional work directly in form of mutual information I gained during the measurement, so that  $W_{max} = -(\Delta E - T\Delta S) + k_B T I$ . It has further been shown [602] that quantum correlations from separated entangled particles can be harnessed to produce mechanical work.

Experimental work on quantum Maxwell demons has also begun, including a superconducting qubit with a microwave cavity demon [603] and photonic light pulses with a demon in the form of a photodetector with feed-forward operation [604]. More recently, a quantum Maxwell demon has been demonstrated out of thermal

equilibrium [605]. In the non-equilibrium domain, fluctuations of thermodynamic quantities become important, so additional entropy is produced, decreasing thermodynamic efficiency. Non-equilibrium effects will become increasingly important as devices approach the nanoscale and become more susceptible to thermal and quantum fluctuations. The understanding of fluctuations of systems in thermal equilibrium was pioneered by Maxwell, Boltzmann and Gibbs. Extending this to nearequilibrium systems was developed by Onsager, Green, and Kubo. However, in recent years, exact non-equilibrium quantum fluctuations results have been obtained by Jarzinski and Crooks [606] [607]. In addition to fabricated devices, biology offers systems that intrinsically operate as non-equilibrium systems. By ingesting nutrients, oxygen, and photons, living organisms maintain themselves by controlling energy and increasing the entropy of their surroundings.

In the equilibrium examples of open quantum systems, the system is in contact with a heat bath which establishes the temperature *T*. The heat bath is a source of stochasticity and irreversibility. More recent works on quantum Maxwell demons have attempted to replace the heat bath with the measurement process itself as the primary source of stochasticity, i.e., a "thermodynamics without bath" [608] [609] [610]. The motivation in these works has not been to understand the measurement problem but to determine the energy expenditure for measurements during quantum computing and error correction. Understanding the physical energy cost for projective measurements would determine the fundamental physical limitation to quantum computers in a way similar to the Landauer limit for classical computers. These works find that the system energy change incurs an additional expense due to the average entropy decrease. It might be thought that the energy cost for a measurement is just the energy difference.

$$\Delta E_S = \mathrm{Tr}[H_S(\dot{\rho}_S - \rho_S)]$$

where  $H_S$  is the system Hamiltonian and  $\dot{\rho}_S = \sum p_k \dot{\rho}_{S,k}$  is the average postmeasurement state and the  $p_k$  are the respective probabilities. However, a computational scenario will include steps similar to that of a Maxwell demon or a heat engine, involving storing the outcomes in a memory for readout and feedback. In addition, the same measurement device will be used repeatedly so that it needs to be restored to the initial state and reset. This will incur additional energy expenses in terms of the average entropy decrease. For projective measurements, the entropic decrease simply takes the form of a Shannon entropy:

$$E_{\text{proj}} = \Delta E_S - k_B T \sum_k p_k \ln p_k$$

Any attempts by Maxwell demons to intervene in irreversible processes appear to be vanquished by Landauer's principle classically and at least in some cases quantum mechanically. Although the validity of Landauer's principle has been experimentally confirmed, perhaps it is not a necessary element in order to address Maxwell's demon in all situations. There have been arguments by Earman and Norton that there may be no need to exorcise the demon if it's assumed from the outset that the demon is governed by the laws of thermodynamics [611] [612]. Bennett, who had proposed using Landauer's principle to exorcize Maxwell's demon, states [613]:

# See the print edition of The Quantum Measurement Problem for quotation.

If the demon is assumed to be a thermodynamic system already governed by the Second Law, no further consideration is needed to ensure that the Second Law is obeved by the entire system and demon. Conversely, if the demon is not assumed to obey the Second Law, no supposition about the entropy cost of information processing can save the Second Law from the demon. Bennett has shown that with classical reversible information processing, i.e., where measurement is equivalent to copying, the act of information destruction in Landauer erasure has a cost exactly sufficient so that the Second Law is obeyed. Theoretical studies of the thermodynamic costs of quantum operations [614] find that the Landauer limit, at which computation becomes thermodynamically reversible, can be reached by classical systems but that for quantum systems there is an unavoidable excess heat generation that results in an inherent thermodynamic irreversibility. This quantum limit, however, applies to quantum computations that are represented as unitary operations that can always be run in reverse. The excess heat generation in this unitary case results from the nocloning theorem, which prevents simply saving a copy of the output before reversing the computation. This prevents a quantum generalization of Bennett's procedure for the reversible unitary case. However, it has not yet been experimentally determined whether the measurements that Maxwell demons carry out in quantum systems are unitary or non-unitary. As discussed in Chapters 3 and 4 of this book, distinguishing unitary from non-unitary processes can be experimentally determined and is a key aspect of the quantum measurement problem. In particular, the understanding of Maxwell's demon at a more fundamental level requires solution of the measurement problem.

Other quantum phenomena might also be considered as quantum demons in the sense that they intervene in quantum measurements but can be distinguished from the Maxwell demons since they do not involve a thermodynamic cycle. One example is *Wigner's Friend*, in which an intelligent *friend* who intervenes as Wigner attempts to carry out a measurement [217]:

## See the print edition of The Quantum Measurement Problem for quotation.

At what point in the measurement do the interference fringes of the wave function disappear, either for the friend or for Wigner: when the friend makes the observation or when he communicates the result to Wigner or when it is registered in Wigner's consciousness? And how does the thermodynamics of the friend intervene in the measurement? These are the typically recurring questions that require a theory of measurement in order to resolve them. If a demon requires measurement to open and close the hole in the diaphragm, then the resolution to the measurement problem can be expected to have an impact on the theory of thermodynamics.

Another process which could be viewed in terms of a quantum demon is the delayed-choice quantum eraser experiment. This originated in the continued attempt to understand the wave-particle duality as argued by Bohr and Einstein in the 1920-30s. An appropriate detector placed in one of the paths of a photon beam splitter is able to destroy the interference pattern, exemplifying Bohr's concept of complementarity. In some cases, this could often be explained as the result of uncontrollable momentum kicks to the quantum particle as quantified by Heisenberg's uncertainty principle. However, it was argued by Scully, Englert, and Walther [615] in 1991 that distinguishing paths could be accomplished solely using quantum entanglement even if no significant momentum kicks were present. The proposal resulted in heated debates in the literature. However, the concept was realized in experiments by Dürr, Nonn, and Rempe [314] in 1996 using beams of cold atoms diffracted by standing waves of light, which demonstrated that they could simply encode within the atoms the information as to which path was taken. This tagging of information is sufficient to cause the interference fringes to disappear entirely even without the presence of momentum kicks. The initially imposed atomic momentum distribution leaves an envelope pattern that was found not to be distorted at the location of the detector showing that momentum kicks cannot be responsible for destroying interference. Instead, the quantum entanglement between the atom's momentum and its internal state result in the attachment of a distinguishable atomic label to the path taken by the atom. The result is that the total atomic-plus-path wave function along one path is orthogonal to that along the others and so the paths can't interfere. However, the entanglement also results in an alternative way for distinguishing paths and destroying interference fringes.

### See the print edition of The Quantum Measurement Problem for figure Figure 5.23: Delayed Choice Quantum Eraser. Shutters separate photons into two cavities. Detector wall absorbs photon and acts as a demon-like photodetector. Solid line with demon erasure, dashed line without [618].

The demonstrated experimental ability to utilize entanglement to distinguish interference paths led to a realization of the *delayed-choice quantum eraser* which had previously been proposed by Scully and Drühl in 1982 [616]. In the quantum eraser, the presence of information accessible to an observer and the subsequent *erasing* of this information, which we might view as being carried out by a demon, qualitatively changes the outcome of an experiment. Combined with John Wheeler's *delayed choice* [617] arrangement, the erasure by the demon can even take place long after the measurement has occurred. The quantum eraser is simply a device in which coherence is lost in a subset of the system but in which the coherence can be restored if a demon erases the tagging information which originally caused the interference to disappear. For a particle sent into a two-slit experiment in which one "tags" which slit the particle goes through, then the interference pattern will disappear. But if one makes the which-slit tag information in-principle unobservable, the interference pattern can be restored. In an example proposed by Scully and Walther [618], Figure 5.23, atoms are detected one-by-one at the screen and interference is observed depending on the

information provided by the detector in the center (i.e., the demon) between the microwave cavities. As long as this demon information still exists, the experimenter can choose to analyze his data in ways that will show fringes or not.

Preskill has proposed an explanation in [619] for which the quantum eraser is understood by realizing that Alice's state  $\rho_A$  is not the same as  $\rho_A$  accompanied by the information Alice has received from the demon. The information provided by the demon changes the physical description of Alice's particle. If Alice's state is the mixed state ensemble  $\rho_A = I/2$ , it is not possible for her to observe interference between states such as  $|\uparrow_z\rangle_A$  and  $|\downarrow_z\rangle_A$  (sum of the solid and dashed curves in Figure 5.23). However, if the demon provides her with the which-way information he has previously collected, Alice can select a sub-ensemble of her spins that are all in the pure state  $|\uparrow_z\rangle_A$  which can now reveal an interference pattern (solid curve in Figure 5.23). The information from the demon can even be delayed an arbitrarily long time, resulting in a delayed-choice quantum eraser. If Alice and demon are space-like separated, there is no invariant meaning as in what order these events occurred. Alice could measure all of her spins long before the demon decides to intervene. This simply reveals that in cases where their correlations are due to quantum entanglement, the situation is completely symmetric between Alice and demon [303].