CHAPTER 5 MAXWELL'S DEMON¹

In 1867 James Clerk Maxwell suggested that a sentient being capable of observing molecular motions might be able to bring about a violation of the second law of thermodynamics through a systematic sorting of molecules. Since then this being, dubbed Maxwell's demon by Lord Kelvin, has been an active topic of scientific inquiry and speculation. Numerous variations of the demon have appeared, some sentient, some automated, some sorting molecules to achieve a temperature difference, some trapping molecules to achieve a pressure difference, and some tending an engine operating on a one-molecule working fluid. Likewise, various concepts have been developed in order to reconcile the demon's actions with the second law. Details of these schemes and concepts may be found in the recent book by Leff and Rex² who have ably traced the demon's history and have identified three epochs. These can be characterized in terms of the dominant explanatory concept.

During the first epoch discussions centering on Maxwell's demon undoubtedly contributed to the much-needed shaping and sharpening of statistical concepts as applied to the molecular description of matter. Toward the end of this epoch, the consensus seemed to be that automated demons will not function, but sentient demons might pose a threat to the second law.

The second epoch began in 1929 with Szilard's³ demon-assisted, one-molecule heat engine. Szilard believed it necessary to introduce the concept of entropy of information in order to prevent this engine from violating the second

¹ Most of this chapter is taken from B.G. Kyle, *Chem. Eng. Ed.*, 29(2),94 (1995).

² H.S. Leff and A.F. Rex, *Maxwell's Demon: Entropy, Information, Computing*, Princeton University Press, Princeton, 1990.

 $^{^{3}}$ L. Szilard, *Z.F. Physik*, 53 840 (1929) [and p. 124 of reference 2].

law. Somewhat later, Brillouin⁴ elaborated on this concept and proved that sorting demons could not beat the second law. He showed that the entropy associated with the measurements a demon would be required to make in order to enable sorting would more than compensate for any entropy reduction brought about by sorting. Therefore the isolated system, including the demon, would show a positive entropy change in conformance with the second law. Later, Denbigh⁵ was able to demonstrate the same result using a classical thermodynamic analysis without recourse to the entropy of information concept. At this point, only Szilard's engine seemed to threaten the integrity of the second law.

In the third and current epoch, the threat of Szilard's one-molecule engine survives. As a rescuing concept, entropy of information seems to have yielded to the idea of memory erasure deriving from the application of thermodynamic ideas to computing.⁶

We will now apply the methods of classical thermodynamics to show that Szilard's engine does not threaten the second law. Also, we will show that current ideas concerning the thermodynamics of computing are unsound.

5.1 SZILARD'S ONE-MOLECULE HEAT ENGINE

In the sixty-four years since its inception, Szilard's one-molecule engine has undergone many modifications, however, since the working principle remains unchanged, the following account patterned after that of reference 1 will be given here.

⁴ L. Brillouin, *J. Appl. Phys.*, *22* 334 (1951) [and p. 134 of reference 2].

⁵ K. Denbigh, *Chem. Brit.*, 17 168 (1981) [and p. 109 of reference 2].

⁶ C.H. Bennett, *Sci Am.*, *255(11)*, 108 (1987) and R. Landauer, *IBM J. Res. Dev.* 5 183 (1961) [and p. 188 of reference 2].

- Step 1. A cylinder containing the one-molecule "gas" is partitioned into halves by the insertion of a partition.
 - Step 2. The Maxwell demon determines which half contains the molecule.
- Step 3. The partition is replaced by a piston. Depending on which half contains the molecule, the piston is suitably connected to a load and the "gas" in expanding moves the piston to the end of the cylinder. Work is done and the "gas" receives heat from a constant-temperature heat bath so that its temperature remains constant. The "gas" now has the same volume and temperature it had initially and the three-step cycle can be repeated.

Szilard reasoned that the cycle would return the "gas" to its original state with no net entropy change, but that the heat bath would have transferred a quantity of heat to the "gas" equal to the work done in step 3 and therefore would have suffered a negative entropy change. In order to insure that the entropy change of the universe not be negative, Szilard proposed the existence of an entropy of information which would be positive and large enough to offset the negative entropy change of the heat bath. It appears that Szilard was the first to quantify entropy of information and he is often credited with originating information theory.

Aside from the obvious operating difficulties that are waved away by invoking frictionless and weightless engine parts, there are two troublesome aspects of Szilard's analysis: The lack of significance of terms such as entropy and temperature as applied to one-molecule "gas" and inconsistency in the thermodynamic analysis. Statistical mechanics tells us that temperature and entropy have meaning only when applied to large collections of molecules and therefore would lack significance when applied to a one-molecule "gas." However, disquieting this may be, stronger grounds for rejecting Szilard's analysis can be found in the failure to maintain a state-specific approach.

Szilard identified the terminal states in analyzing step 3, but abandoned the state perspective in analyzing step 1. In step 3 he reasoned that a quantity of 1/N mol of "gas" (assumed ideal) expands isothermally and doubles its volume doing

work $(1/N)RT\ln 2$ (= $kT\ln 2$) and receiving an equal quantity of heat from the heat bath. For step 1 it is merely stated that a partition is inserted with no consideration of the physical ramifications. Because the density of a real gas is uniform, the insertion of a partition would only divide the gas into two identical halves. Not so for a one-molecule gas! The proper description of step 1 is that initially the "gas" occupies the volume *V* with a pressure *P* while the final state consists of the "gas" occupying a volume V/2 with a pressure 2P with a vacuum in the remaining volume V/2. Obviously to bring about this change in state requires the expenditure of work. If the process were reversible and isothermal, the work of compressing the "gas" from V to V/2 would be kTln2. An equal quantity of heat would be delivered to the heat bath. The result of the 3-step cycle would be no net work performed and no net heat transfer. Breaking even is the best that can be expected with this cycle. As the insertion of a partition hardly qualifies as a reversible process, the input work and, concomitantly, the heat rejected to the heat bath would be expected to exceed kTln2 with the net result of the cycle being the conversion of work into heat. There is no need to conjure up a compensating entropy of information in order to save the second law from the one-molecule heat engine!

This same result can be obtained if a microscopic perspective is consistently applied. Entropy changes for the "gas" corresponding to its volume changes can be calculated from the Sackur-Tetrode equation for steps 1 and 3; these will be equal but opposite in sign. For a reversible cycle, there are corresponding entropy changes in the heat bath which are also equal and opposite in sign, hence no net extraction of heat and therefore no second law violation.

The preceding argument takes its impetus from the statement of Jauch and Báron⁷ that "the idealizations in Szilard's experiment are inadmissible" as "the gas

 $^{^7}$ J.M. Jauch and J.G. Báron, *Helv. Phys. Acta*, 45, 220 (1972) [and p. 160 of reference 2].

violates the law of Gay-Lussac because the gas is compressed to half its volume without expenditure of energy." It is unfortunate that this fatal flaw was identified in 1972 but seems to have been ignored by later workers. The only exception seems to have been an attempted rebuttal of Jauch and Báron by Costa de Beauregard and Tribus⁸, however, these authors offered arguments that can only be described as oblique and bizarre.

In passing, it should be noted that had Szilard's analysis been correct, the contrivance of an entropy of information would have balanced the entropy but would not have saved the second law in its most basic form. Unless heat dissipation is associated with the entropy of information, there would still have been a complete conversion of heat into work. Szilard offered no details concerning the manifestation of this entropy change.

5.2 THE THERMODYNAMICS OF COMPUTING

Despite the exposure by Jauch and Báron of the flaw in Szilard's engine, work dedicated to saving the second law has continued apace with the computer now assuming the role of savior. Instead of the "corrective" $k\ln 2$ entropy units being assigned to information acquisition, the idea has now been advanced that these units of entropy must be assigned to memory erasure. This is purported to be the entropy change accompanying the thermodynamically reversible erasure of one bit of information. The argument proceeds by stating that a measurement in the one-molecule heat engine can be made reversibly (no creation of entropy) but after the completion of a cycle the demon must reset its memory at a cost of $k\ln 2$ units of entropy increase in the surroundings due to heat dissipation. As the work

⁸ O. Costa de Beauregard and M. Tribus, *Helv. Phys. Acta*, *47*, 238 (1974) [and p. 173 of reference 2].

⁹ C.H. Bennett, Sci. Am., 255(11), 108 (1987).

¹⁰ R. Landauer, *IBM J. Res. Dev.*, 5, 183 (1961) [and p. 188 of reference 2].

of Landauer¹¹ forms the basis for this explanation, it will now be subjected to a critical review.

Borrowing ideas from thermodynamics, statistical mechanics, and information theory, Landauer obtained an expression for the minimum energy dissipation in a computer. His system was an assembly of N bits each of which could occupy either a zero or a one state. He assumed each state to have the same entropy and considered a restore-to-one operation where the bits, initially randomized with regard to state, were all set to one. Arguing that the number of states available to a bit had been reduced from two (either zero or one) to one in the process, he reasoned that the entropy of each bit would be reduced by $k\ln 2$. He continued by stating that the entropy decrease of a bit must be compensated by heat dissipation to the surroundings of a least $k\ln 2$. Despite disclaiming a reliance on information theory, Landauer obviously views the entropy change of $k\ln 2$ per bit in that context.

Landauer is not justified in assigning an entropy change to the process of restore-to-*one*. Although he provides little explanation, he seems to be applying methods of statistical mechanics, not at the molecular level, but to a system comprised of *N macroscopic* subsystems, the bits. Not only is this procedure not permissible, but the process considered has no thermodynamic significance. Landauer's restore-to-*one* process involves macroscopic subsystems and is akin to calculating the entropy change between different arrangements of pieces on a checkerboard.

Each bit will exhibit a set of intensive properties which will depend only on the state-determining intensive variables (e.g., temperature and intensity of magnetization). In terms of intensive properties, each bit behaves as if it alone were present and oblivious of the identity of its neighbors. Because Landauer set entropies equal for states *zero* and *one*, there can be no thermodynamically significant entropy change in going between any two spatial configurations of *zeros*

¹¹ ibid

and *ones*. Of course, if the transition between states is not carried out reversibly, as would be expected of a computer, heat dissipation to the surroundings will account for the necessary entropy increase of the universe.

Landauer seems to view $k\ln 2$ as the information entropy of a bit, however, as indicated in § 6.3 and more convincingly shown by Denbigh and Denbigh¹², information entropy does not reduce to thermodynamic entropy. Landauer's inclusion of the $k\ln 2$ term in an entropy balance is therefore inadmissible.

For Landauer's assumption of equal entropies for states *zero* and *one*, a legitimate thermodynamic analysis shows that there would be no entropy change in the surroundings from a thermodynamically reversible resettling of memory. This would contribute no additional entropy changes to the analysis of Szilard's engine but, as we have seen, none is needed.

The concept of information entropy has proven useful in the field of communication theory and perhaps a specially defined "entropy" will prove useful for computer design and programming. Nevertheless, neither quantity has thermodynamic significance and neither is necessary to save the second law from the assault of a Maxwell demon.

¹² K.G. Denbigh and J.S. Denbigh, *Entropy in Relation to Incomplete Knowledge*, Cambridge University Press, Cambridge, 1985.