Lenard’s theorem

Lenard essentially demonstrated the following statement quantum mechanically:\textsuperscript{1}

The second law of thermodynamics $\iff$ The equilibrium distribution is a monotone decreasing function of energy.

If $\rho(0) = \sum_n |n; 0\rangle w(E_n(0)) \langle n; 0|$, with $w(x)$ being a decreasing function of $x$, then

$$\langle H \rangle_U - \langle H \rangle_0 \geq \langle H \rangle_{ad} - \langle H \rangle_0,$$

where $\langle \cdot \rangle_0$ is the expectation value with respect to the initial distribution $\rho(0)$, and $\langle \cdot \rangle_U$ is the average over $U \rho(0) U^*$ for an arbitrary unitary operator $U$, and $\langle \cdot \rangle_{ad}$ implies the average over the distribution reached from $\rho(0)$ by a quantum mechanical adiabatic process. If the initial and the final Hamiltonians are identical (1) becomes Planck’s principle under isolation condition.

†An outline of the proof of (1)

Let us assume that eigenvalues are ordered as $E_i(\lambda) \leq E_{i+1}(\lambda)$. Let the initial distribution be $\rho_0 = \sum_n |n; 0\rangle w(E_n(0)) \langle n; 0|$. We have only to show that if $w(x)$ is nonincreasing as a function of $x$, for any unitary transformation $U$,

$$\text{Tr}(HU\rho_0 U^{-1}) \geq \langle H \rangle_{ad}. \quad \text{(2)}$$

In terms of components this reads

$$\sum_{nm} E_n(1) P_{nm} w(E_m(0)) \geq \sum_n E_n(1) w(E_n(0)). \quad \text{(3)}$$

where $P_{nm}$ is the doubly stochastic matrix already given in (??). Therefore, if we can show the following inequality, we are done: Let $A_i$ and $B_i$ be both increasing sequences. Then, for any doubly stochastic matrix $P_{ij}$

$$\sum_{ij} P_{ij} A_i B_j \leq \sum_i A_i B_i. \quad \text{(4)}$$

To prove this we have only to find an operation $Q$ such that $A^T P B \leq A^T (QP) B$ and $Q^n P = I$ for some finite positive $n$.\textsuperscript{2} Let $P$ be an $N \times N$ matrix with nonzero elements $P_{ab}$ and $P_{ai}$ for some $a, b (a, b \in \{1, \cdots, N\}$; if there is no such pair replace $N$ with $N - 1$ and repeat the argument here). $Q$ is a procedure to find such a pair $a, b$ and change the


\textsuperscript{2}The proof here is due to Nir Friedman (private commun., 2008).
following four elements $P_{aN}, P_{Nb}, P_{NN}, P_{ab}$ as follows. Let the smaller one of $P_{aN}$ and $P_{Nb}$ be $\Delta$: $\Delta = \min\{P_{aN}, P_{Nb}\}$:

\[
(QP)_{aN} = P_{aN} - \Delta, \\
(QP)_{Nb} = P_{Nb} - \Delta, \\
(QP)_{ab} = P_{ab} + \Delta, \\
(QP)_{NN} = P_{NN} + \Delta.
\]

Then,

\[
A^T(QP)B - A^T PB = (A_a - A_N)(B_b - B_N)\Delta \geq 0.
\]

$QP$ remains to be a doubly stochastic matrix, and at least one element in the $N$-th raw or column goes from a positive value to zero. Repeat applying $Q$ until there is no pair $a, b$ such that $P_{aN}$ and $P_{Nb}$ are simultaneously nonzero. Within finitely many application of $Q$ all the elements of the $N$-th raw and column become zero except for $P_{NN} (= 1)$. Thus, the problem has been reduced to a $N - 1 \times N - 1$ problem. Since the theorem is trivial for $N = 1$, we are done.

Conversely, the second law implies that $w(x)$ must be decreasing. If the fourth law of thermodynamics is also assumed, $w(E) \propto e^{-\beta E}$ follows with some ‘technical’ conditions. More precisely, the assumptions are:

(i) **Passivity**: This is essentially the second law. Let $H(t)$ be a time-dependent Hamiltonian and the density operator $\rho(t)$ obeys von Neumann’s equation

\[
i\hbar \frac{d\rho}{dt} = [H(t), \rho].
\]

Here, we assume that this Hamiltonian has no time dependence outside the range of time $[0, 1]$ and $H(0) = H(1)$. Then, the work needed for this cycle is nonnegative:

\[
W(K, \rho_0) = \int_0^1 dt \text{Tr}\rho(t)\frac{dH(t)}{dt} \geq 0.
\]

(ii) **Structural stability**: any small perturbation of the Hamiltonian does not destroy the system passivity.

(iii) Let a compound system consist of two subsystems and be in a passive structurally stable state. Its density operator is the product\(^3\) of the density operators of the two subsystems.

Roughly speaking, (i) implies that the distribution is a monotone decreasing function of

\(^3\text{More precisely, tensor product}\)
energy, and (iii) restricts the functional form to be exponential. Consequently, the canonical distribution is derived. If we do not demand (iii), more general distributions could be obtained.

Lenard’s equivalence relation sounds plausible, even if the isolation condition is replaced with the thermodynamic adiabatic condition. However, thermodynamic adiabatic conditions lack mechanical interpretation, so such a thermodynamically meaningful assertion can never be proved by mechanics. Furthermore, the mechanical interpretation of work follows the tradition initiated by Einstein, and pays no attention to whether it is macroscopically realizable or not. In short, we do not have any understanding of heat in terms of mechanics, so no satisfactory relation between the second law and statistical mechanics is obtained.