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Addendum to "Waiting for Landauer"
Units in the one-molecule gas – piston system.

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Overview

The Problem

In my paper "Waiting for Landauer," Section 7.5 illustrates the general no-go result of Section 7.4 with the example of a one-molecule gas that expand isothermally while working against a piston. The piston resists the one-molecule gas pressure in a way that maintains equilibrium throughout the expansion. This requires that the piston not press down on the gas as it would in an ordinary gravitational field. It requires a novel field specifically tuned to maintain the equilibrium.

G. Baris Bagci has pointed out in a private communication[1] that the Hamiltonian presumed for the piston has inconsistent units. That is, the piston Hamiltonian is

$$E_{pist}(\mathbf{x}, \boldsymbol{\pi}) = 2kT \ln x + \pi^2/2M \tag{1}$$

where M is the piston's mass and $\mathbf{x} = (x,y,z)$ and $\boldsymbol{\pi} = (\pi_x, \pi_y, \pi_z)$ are the piston's canonical position and momentum. T is the gas temperature, which enters here purely as an arbitrarily set parameter in the Hamiltonian. The difficulty is that E_{pist} must have units of energy. The second

[1] "You should not sleep until this problem is solved."

term in (1) has them. It is $\pi^2/2M$ = "(linear momentum)^2/ mass," which is equivalent to energy in units. The first term does not have them. It is 2kT ln x. The first term in the product, 2kT, already has the units of energy. The second, ln x, introduces an additional dependency on the unit chosen for length. For example, if the coordinate distance x is measured in millimeters or meters, there will be a difference in the ln x term of $\ln(10^3)$, since the factor 10^3 scales between millimeter and meter measurements.[2]

The Solution

The Hamiltonian (1) is incomplete. To render it consistent in units, we need to add an arbitrary length constant λ whose effect is to set a length scale. It is introduced through the modification to the Hamiltonian of (1) as

$$E_{pist}(\mathbf{x}, \boldsymbol{\pi}) = 2kT \ln (x/\lambda) + \pi^2/2M \tag{2}$$

The modified term $\ln (x/\lambda)$ is now independent of the unit of length chosen and the units in the modified Hamiltonian are consistent.

Fortunately this modification does not affect the results derived for the system in Section 7.5. This follows from the fact that

$$\ln (x/\lambda) = \ln x - \ln \lambda$$

That entails that the modification merely adds a constant term to the Hamiltonian (1) that can be rewritten as

$$E_{pist}(\mathbf{x}, \boldsymbol{\pi}) = 2kT \ln x + \pi^2/2M - 2kT \ln \lambda$$

The λ dependent constant term drops out of the calculations, having no effect in the final results, which are independent of the particular value chosen for λ. The results employing (1) can simply be thought of as results derived for the special case of $\lambda = 1$ in the chosen set of units. The results would be the same if we had instead chosen $\lambda = 2$ or $\lambda = 3$ or any other non-zero value.

The discussion below will demonstrate these last claims.

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[2] This awkward means of expressing unit dependence is needed. The usual method of identifying units in terms of M (mass), L (length) and T (time) does not apply directly here. A quantity that has units L, for example, should scale linearly in a change of unit of length. The term ln x does not scale this way with changes in the unit of length, but it is still unit dependent.

Partition Function

The first relevant computation in Section 7.5 is the computation of the partition function of the piston. In that computation it is assumed that the momentum $\boldsymbol{\pi}$ can take on all values; that the y and z coordinates vary over some very narrow area A (= the area swept by the tiny amount of sideways motion possible for the piston); and that the x coordinate varies from h to ∞. We have for the partition function

$$Z_{pist}(h) = \int_{all\ \ \pi,y,z} \int_{x=h,\infty} \exp\left(-\frac{2kT\ln(x/\lambda) + \pi^2/2M}{kT}\right) d\pi dydzdx \qquad (3)$$

In the paper, I did not explicitly compute all the terms in the integral, since most of them do not appear in the final results and it would have cluttered the paper with unnecessary formulae. However for completeness I can provide them here. This last expression (3) is a product of three integrals:

$$Z_{pist}(h) = I_1\ I_2\ I_3$$

where

$$I_1 = \int_{x=h,\infty} \exp\left(-\frac{2kT\ln(x/\lambda)}{kT}\right) dx = \lambda \int_{x=h,\infty} \exp(-2\ln(x/\lambda)) d(x/\lambda) = \lambda \int_{x=h,\infty} (x/\lambda)^{-2} d(x/\lambda)$$

$$= \lambda\left[-\frac{\lambda}{x}\right]_{x=h,\infty} = \frac{\lambda^2}{h}$$

$$I_2 = \int_{all\ \ y,z} dydz = A$$

$$I_3 = \int_{all\ \ \pi} \exp\left(-\frac{\pi^2}{2MkT}\right) d\pi$$

$$= \left(\sqrt{MkT}\right)^3 \int_{all\ \ \pi} \exp\left(-\tfrac{1}{2}\left(\left(\frac{\pi_x}{\sqrt{MkT}}\right)^2 + \left(\frac{\pi_y}{\sqrt{MkT}}\right)^2 + \left(\frac{\pi_z}{\sqrt{MkT}}\right)^2\right)\right) d\left(\frac{\pi_x}{\sqrt{MkT}}\right) d\left(\frac{\pi_y}{\sqrt{MkT}}\right) d\left(\frac{\pi_z}{\sqrt{MkT}}\right)$$

Writing $t_x = \dfrac{\pi_x}{\sqrt{MkT}}$, etc. we have

$$I_3 = \left(\sqrt{MkT}\right)^3 \int_{all\ \ t} \exp\left(-\frac{t_x{}^2 + t_y{}^2 + t_z{}^2}{2}\right) dt_x dt_y dt_z$$

$$= \left(\sqrt{2\pi MkT}\right)^3 \int_{all\ \ t} \phi(t_x)\phi(t_y)\phi(t_z) dt_x dt_y dt_z = \left(\sqrt{2\pi MkT}\right)^3$$

where $\phi(t)$ is the standard normal distribution whose integral over $(-\infty,\infty)$ is unity.

Combining these last three terms we have for the partition function

$$Z_{pist}(h) = \left(\sqrt{2\pi MkT}\right)^3 \cdot A \cdot \frac{\lambda^2}{h} \tag{4}$$

This expression has the units $(\text{momentum})^3(\text{length})^3$ which are appropriate to an integral over a phase space with canonical volume element $d\pi_x d\pi_y d\pi_z dxdydz$. To see this, note that MkT has units (mass)x(energy), which is equivalent to $(\text{momentum})^2$. Hence $\left(\sqrt{2\pi MkT}\right)^3$ has units $(\text{momentum})^3$. The term $A\lambda^2/h$ has units $(\text{length})^4/\text{length} = (\text{length})^3$.

Hence the partition function (3), (4) associated with the modified Hamiltonian (2) has appropriate units.

The added λ term simply adds a multiplicative constant λ^2 to the expression for the partition function. We shall now see that this added term does not appear in the quantities of physical significance in the example.

Probabilities

The piston's height x is canonically distributed. Consider the probability for the x position of the piston to be in the interval (x_1, x_2), where $h < x_1 < x < x_2 < \infty$. This probability is given by

$$P(x_1,x_2) = \frac{1}{Z_{pist}(h)} \int_{all\ \ \pi,y,z} \int_{x=x_1,x_2} \exp\left(-\frac{2kT\ln(x/\lambda) + \pi^2/2M}{kT}\right) d\pi dydzdx \tag{5}$$

This integral is similar in structure to the integral of the normalizing partition function (3). A comparison of that integration with expression (5) reveals that the integrals in (5) corresponding to integrals I_2 and I_3 above are the same as those in (3) and thus cancel out. We are left only with two terms corresponding to the integral in I_1. That is

$$P(x_1,x_2) = \frac{\lambda/x_1 - \lambda/x_2}{\lambda/h} = h(1/x_1 - 1/x_2) \tag{6}$$

This formula yields probabilities in the range of 0 to 1 as expected. More importantly, the length scale parameter λ has disappeared. It does not influence the probability distribution. The reason, as noted earlier, is that it contributes an additive constant to the Hamiltonian (1). That in turn appears as a multiplicative constant in the integrals (3) and (5) and it cancels out.

Free Energy

The second important quantity computed is the free energy of the gas piston, which is computed in the paper with the canonical formula relating the free energy F of any system to its partition function Z

$$F = -kT \ln Z \tag{7}$$

While this is a standard result reported in the textbooks, one can see that the general formula is inconsistent as far as units are concerned. Free energy has units of energy. The first term in the canonical expression, kT, already has units of energy. The second term ln Z will be dependent on the units used for momentum and length in computing the partition function Z.

This inconsistency results from a common short cut in the formula and it is readily remedied. The formula (7) is incomplete. It gives the value of the free energy only with respect to some arbitrarily chosen reference state. The incomplete expression is adequate for the analysis of the paper, since changes of free energy are all that enter into the consideration of equilibrium and thermodynamic forces.

To recover the correct and full expression and display consistency in the units, we need to restore this reference state. Let us assume that the reference state has free energy F_0 for a state with partition function Z_0. Then we have as the correct formula

$$F = -kT \ln (Z/Z_0) + F_0 \tag{8}$$

Since Z/Z_0 has no units, the free energy F of (8) has the units of energy of kT.

Substituting the expression for the partition function (4) into the expression for free energy

$$F_{pist}(h) = -kT \ln(Z_{pist}(h)/Z_0) + F_0$$

we recover

$$F_{pist}(h) = -kT \ln\left[\frac{\left(\sqrt{2\pi MkT}\right)^3 \cdot A \cdot \dfrac{\lambda^2}{h}}{Z_0}\right] + F_0 \tag{9}$$

The units in this equation are consistent since it is simply a version of (8).

We can also see that the constant λ contributes an additive constant to the free energy and thus will play no role in the subsequent calculations:

$$F_{pist}(h) = -kT\ln\left[\frac{\left(\sqrt{2\pi MkT}\right)^3 \cdot A \cdot \frac{1}{h}}{Z_0}\right] - kT\ln\left[\lambda^2\right] + F_0 \qquad (10)$$

Generalized Force

The generalized force that the piston applies to the one-molecule gas is computed by taking the partial derivative of the free energy (10) with respect to the parameter h:

$$X_{pist}(h) = -\left.\frac{\partial}{\partial h}\right|_T F_{pist}(h) = -\frac{kT}{h} \qquad (11)$$

This simplification depends upon the h dependency of the piston free energy in (10), which can be rewritten as

$$F_{pist}(h) = -kT \ln(1/h) + \text{constant}(T) = kT \ln h + \text{constant }(T)$$

The units for the expression for force in (11) are consistent. The formula kT/h has the form (energy)/(length), which has the units of force.

Finally, the parameter λ does not appear in (11) so its value does not affect the force.

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In sum, the addition of the parameter λ to the piston Hamiltonian restores consistency in the units in the formulae, but otherwise does not alter the results of the example as presented in the paper. These results derive from the h dependency of various quantities: the partition function (4) still varies with 1/h; the free energy (1) varies with ln h; and the generalized force (11) is precisely the one needed to balance gas pressure, -kT/h.