Curvature Calculation for f PhL 6.6.15

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6.3 More details of the Boltzmann problem solution

Start with

$$f = \ln\Omega = \Sigma_i [(1+\ln g_i)N_i - N_i \ln N_i] = \Sigma_i N_i [1 + \ln(g_i/N_i)] . \qquad (6.2.3)$$

The constraints $\Sigma_i N_i = M$ and $\Sigma_i N_i \varepsilon_i = U$ can be regarded as two equation in the two unknowns N_1 and N_2 which are easily solved to obtain,

$$\begin{aligned} N_1 &= +(\varepsilon_2 - \varepsilon_1)^{-1}[\varepsilon_2 M - U + \Sigma_{n=3}^{m} (\varepsilon_i - \varepsilon_2)N_i] &&= N_1(N_3, \ldots N_m) \\ N_2 &= -(\varepsilon_2 - \varepsilon_1)^{-1}[\varepsilon_1 M - U + \Sigma_{n=3}^{m} (\varepsilon_i - \varepsilon_1)N_i] &&= N_2(N_3, \ldots N_m) . \end{aligned} \qquad (6.3.1)$$

Notice that, for i = 3,4...m,

$$\begin{aligned} \frac{\partial N_1}{\partial N_i} &= +(\varepsilon_2 - \varepsilon_1)^{-1} [(\varepsilon_i - \varepsilon_2)] = \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} \\ \frac{\partial N_2}{\partial N_i} &= -(\varepsilon_2 - \varepsilon_1)^{-1} [(\varepsilon_i - \varepsilon_1)] = -\frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} . \end{aligned} \qquad (6.3.2)$$

Now think of f as function of $N_3,,,,N_m$,

$$f(N_1(N_3, \ldots N_m), N_2(N_3, \ldots N_m), N_3, \ldots .N_m) . \qquad (6.3.3)$$

Compute the total derivative df/dN_i for i = 3,4...n:

$$\begin{aligned} \frac{df}{dN_i} &= f_1 \frac{\partial N_1}{\partial N_i} + f_2 \frac{\partial N_2}{\partial N_i} + f_i \qquad \text{where } f_i \equiv \frac{\partial f}{\partial N_i} \\ &= f_1 \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} - f_2 \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} + f_i \qquad (6.3.2) \\ &= \ln(g_1/N_1) \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} - \ln(g_2/N_2) \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} + \ln(g_i/N_i) \qquad (6.2.6) \end{aligned} \qquad (6.3.4)$$

Installing the solution values $\ln(N_i/g_i) = \lambda_1 + \lambda_2 \varepsilon_i$ shown in (6.2.8) this becomes

$$= (\lambda_1 + \lambda_2\varepsilon_1)\,\frac{\varepsilon_i-\varepsilon_2}{\varepsilon_2-\varepsilon_1} - (\lambda_1 + \lambda_2\varepsilon_2)\frac{\varepsilon_i-\varepsilon_1}{\varepsilon_2-\varepsilon_1} + (\lambda_1 + \lambda_2\varepsilon_i)$$

$$= \lambda_1 \left[\frac{\varepsilon_i-\varepsilon_2}{\varepsilon_2-\varepsilon_1} - \frac{\varepsilon_i-\varepsilon_1}{\varepsilon_2-\varepsilon_1} + 1\right] + \lambda_2 \left[\varepsilon_1\frac{\varepsilon_i-\varepsilon_2}{\varepsilon_2-\varepsilon_1} - \varepsilon_2\frac{\varepsilon_i-\varepsilon_1}{\varepsilon_2-\varepsilon_1} + \varepsilon_i\right]$$

$$= \lambda_1 \left[\frac{\varepsilon_i-\varepsilon_2}{\varepsilon_2-\varepsilon_1} - \frac{\varepsilon_i-\varepsilon_1}{\varepsilon_2-\varepsilon_1} + \frac{\varepsilon_2-\varepsilon_1}{\varepsilon_2-\varepsilon_1}\right] + \lambda_2 \left[\varepsilon_1\frac{\varepsilon_i-\varepsilon_2}{\varepsilon_2-\varepsilon_1} - \varepsilon_2\frac{\varepsilon_i-\varepsilon_1}{\varepsilon_2-\varepsilon_1} + \varepsilon_i\frac{\varepsilon_2-\varepsilon_1}{\varepsilon_2-\varepsilon_1}\right]$$

$$= \lambda_1 [0] + \lambda_2[0] = 0 \qquad (6.3.5)$$

This is the expected result since the solution is supposed to be a critical point of f given in (6.3.3).

Our main interest is in the second derivative d^2f/dN_i^2 . If this comes out negative at the solution point, we know we have a maximum. Applying d/dN_j to the second line in (6.3.5),

$$\frac{d^2f}{d^2N_i} = \frac{df_1}{dN_i}\frac{\varepsilon_i-\varepsilon_2}{\varepsilon_2-\varepsilon_1} - \frac{df_2}{dN_i}\frac{\varepsilon_i-\varepsilon_1}{\varepsilon_2-\varepsilon_1} + \frac{df_i}{dN_i}$$

$$= \left[f_{11}\frac{\varepsilon_i-\varepsilon_2}{\varepsilon_2-\varepsilon_1} - f_{12}\frac{\varepsilon_i-\varepsilon_1}{\varepsilon_2-\varepsilon_1} + f_{1i}\right]\frac{\varepsilon_i-\varepsilon_2}{\varepsilon_2-\varepsilon_1} \qquad f_{ij} \equiv \frac{\partial^2 f}{\partial N_i \partial N_j}$$

$$- \left[f_{21}\frac{\varepsilon_i-\varepsilon_2}{\varepsilon_2-\varepsilon_1} - f_{22}\frac{\varepsilon_i-\varepsilon_1}{\varepsilon_2-\varepsilon_1} + f_{2i}\right]\frac{\varepsilon_i-\varepsilon_1}{\varepsilon_2-\varepsilon_1}$$

$$+ \left[f_{i1}\frac{\varepsilon_i-\varepsilon_2}{\varepsilon_2-\varepsilon_1} - f_{i2}\frac{\varepsilon_i-\varepsilon_1}{\varepsilon_2-\varepsilon_1} + f_{ii}\right] \qquad i = 3,4....m \qquad (6.3.6)$$

Recall now that

$f = \ln\Omega = \Sigma_i\,[(1+\ln g_i)N_i - N_i \ln N_i]$ *(6.2.3)*

$f_i = \ln g_i - \ln N_i$ *(6.2.6)*

$$f_{ij} = -\,\delta_{ij}(1/N_i) \qquad (6.3.7)$$

Therefore (6.3.6) simplifies to

$$\frac{d^2f}{d^2N_i} = f_{11}\left[\frac{\varepsilon_i-\varepsilon_2}{\varepsilon_2-\varepsilon_1}\right]^2 + f_{22}\left[\frac{\varepsilon_i-\varepsilon_1}{\varepsilon_2-\varepsilon_1}\right]^2 + f_{ii}$$

$$= -\left\{\frac{1}{N_1}\left[\frac{\varepsilon_i-\varepsilon_2}{\varepsilon_2-\varepsilon_1}\right]^2 + \frac{1}{N_2}\left[\frac{\varepsilon_i-\varepsilon_1}{\varepsilon_2-\varepsilon_1}\right]^2 + \frac{1}{N_i}\right\} \qquad (6.3.8)$$

This says that the curvature of f in all independent directions N_i for i = 3,4...m is negative and this is true for *all* vectors $\mathbf{N} = \{N_i\}$. This is of course then true for the solution vector **N**. But for the solution vector **N** we also have $df/dN_i = 0$ from (6.3.5) and therefore the solution is a *maximum* of f and therefore of Ω.

Finally, we may *estimate* the width of the peak of f and then of Ω. The energy fractions in (6.3.8) are on the ballpark order of unity and the N_i are on the order of M, the total number of particles. If we do Taylor expansion of f(**N**) in the i direction only (i = 3,4...m) about the solution **N**, then

$$f(N_i + dN_i) \approx f(N_i) + (df/dN_i)dN_i + (1/2)(d^2f/d^2N_i)\,(dN_i)^2 + ,,,$$

$$= f(N_i) + 0 * dN_i - (1/2)\,\{\frac{1}{N_1}\,[\frac{\varepsilon_i-\varepsilon_2}{\varepsilon_2-\varepsilon_1}]^2 + \frac{1}{N_2}[\frac{\varepsilon_i-\varepsilon_1}{\varepsilon_2-\varepsilon_1}]^2 + \frac{1}{N_i}\}\,(dN_i)^2$$

$$\sim f(N_i) + 0 - (1/2)\,\{\frac{3}{M}\}\,(dN_i)^2 \sim f(N_i) - \frac{1}{M}\,(dN_i)^2$$

so

$$df = f(N_i + dN_i) - f(N_i) \sim -\frac{1}{M}\,(dN_i)^2 \,. \qquad (6.3.9)$$

Therefore,

$$|df| \sim \frac{1}{M}\,(dN_i)^2 \qquad \Rightarrow \qquad dN_i \sim \sqrt{M\,|df|} \qquad \Rightarrow$$

$$\frac{dN_i}{M} \sim \sqrt{\frac{|df|}{M}} \qquad (6.3.10)$$

This gives a rough estimate of the fractional distance one must move in the N_i direction to cause a reduction |df| in f from the peak value of f.

Suppose we are interested in finding dN_i such that the Ω(**N**) drops to half its peak value. Then

$$\Omega_{half}/\Omega_{peak} = 1/2 \qquad \Rightarrow \qquad \ln \Omega_{half} - \ln \Omega_{peak} = 1/2 \qquad \Rightarrow$$

$$f_{half} - f_{peak} = \ln(1/2) \qquad \Rightarrow \qquad df = f_{peak} - f_{half} = \ln(2) = 0.7 \qquad (6.3.11)$$

Then (6.3.10) says

$$\frac{dN_i}{M} \sim \sqrt{\frac{0.7}{M}} = \frac{.83}{\sqrt{M}} \sim \frac{1}{\sqrt{M}} \qquad (6.3.12)$$

For a macroscopic box of gas particles, one might have $M = 10^{20}$ and then $\frac{dN_i}{M} \sim 10^{-10}$. Since this is the fractional half-width of the peak in Ω, the peak is *extremely* sharp. This then is why, in an ensemble of macroscopic particle systems, all systems will have almost the same **N** value.

6.4 A numerical example