Boltzmann Misc support stuff PhL 6.6.15

This was taken from the end of the boltz shot 2 document.

How do we know that our solution $\{N_i\}$ corresponds to a maximum of Ω or f ?

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Consider now the first and second derivatives of f,

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

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

$f_{ii} = -1/N_i$ plots ok

$H = f + \lambda_1 a + \lambda_2 b$ // (6.2.5)

$H_i = f_i + \lambda_1 a_i + \lambda_2 b_i = f_i + \lambda_1 * 1 + \lambda_2 * \varepsilon_i$ // (6.2.6)

$H_{ii} = f_{ii} = -1/N_i$ $R_{curv} = 1/H_{ii} = -N_i$

am happy to here

$\Omega = e^f$

$\Omega_i = \Omega f_i$ plot has peak, is OK

$\Omega_{ii} = \Omega f_{ii} + \Omega_i f_i = \Omega f_{ii} + \Omega f_i^2 = \Omega (f_{ii} + f_i^2) = \Omega (-1/N_i + [\ln(g_i/N_i)]^2)$

$h = \Omega + \lambda_1' a + \lambda_2' b$

$h_i = \Omega_i + \lambda_1' a_i + \lambda_2' b_i = \Omega_i + \lambda_1 * 1 + \lambda_2 * \varepsilon_i$

$h_{ii} = \Omega_{ii}$

Therefore

h_{ii} = curvature of the Ω curve $= \Omega_{ii} = \Omega (-1/N_i + [\ln(g_i/N_i)]^2)$

But this appears to me to be a large *positive* number so the h curve is cupping up which is wrong!

BUT, h_{ii} is not really $\partial^2 h/\partial^2 N_i$ whereas the curvature is given by d^2h/d^2N_i which is a completely different function!

Realization: Consider

$f(N_1,N_2,N_3) = \ln \Omega = \Sigma_{i=1}^{3} [(1+\ln g_i)N_i - N_i \ln N_i]$ // (6.2.3)

The object f_i is a *partial* derivative!

$f_i = \partial f/\partial N_i = \ln(g_i/N_i) = \ln g_i - \ln N_i$

But the curve I am plotting for f which shows the bell shape is this

$$F(N_1) = f(N_1,N_2(N_1),N_3(N_1))$$

The slope of the plot is then

$$dF/dN_1 = \partial f/\partial N_1 + \partial f/\partial N_2 * \partial N_2/\partial N_1 + \partial f/\partial N_3 * \partial N_3/\partial N_1$$

$$= f_1 + f_2(\partial N_2/\partial N_1) + f_3(\partial N_3/\partial N_1) \qquad = \text{slope of the bell curve plot of f}$$

Now I solved to get

$$N_2 = -(\varepsilon_2-\varepsilon_3)^{-1}[(e_1-e_3)N_1 - U + Me_3]$$

$$N_3 = +(\varepsilon_2-\varepsilon_3)^{-1}[(e_1-e_2)N_1 - U + Me_2]$$

Therefore

$$(\partial N_2/\partial N_1) = -(\varepsilon_2-\varepsilon_3)^{-1}[(e_1-e_3) = -(-1)^{-1}(-2) = 2$$

$$(\partial N_3/\partial N_1) = +(\varepsilon_2-\varepsilon_3)^{-1}[(e_1-e_2) = +(-1)^{-1}(-1) = 1$$

Therefore the curve slope is

$$dF/dN_1 = f_1 + 2f_2 + f_3$$

where in all functions we replaced N_2 and N_3 as shown. So this is a far cry from $f_1 \geq$

Continue on this line 6/5/15

Let's think about f or Ω by using the fact that the constraints are simple to just remove two variables and then we have something we can plot and deal with.

Consider

$$N_1 + N_2 + \Sigma_{n=3}^{m} N_i = M$$
$$\varepsilon_1N_1 + \varepsilon_2N_2 + \Sigma_{n=3}^{m} \varepsilon_iN_i = U$$

or

$$N_1 + N_2 = M - \Sigma_{n=3}^{m} N_i$$
$$\varepsilon_1N_1 + \varepsilon_2N_2 = U - \Sigma_{n=3}^{m} \varepsilon_iN_i$$

Solve for N_1 and N_2 as follows

$$\varepsilon_1 N_1 + \varepsilon_1 N_2 = \varepsilon_1 M - \varepsilon_1 \Sigma_{n=3}^{m} N_i$$
$$\varepsilon_1 N_1 + \varepsilon_2 N_2 = U - \Sigma_{n=3}^{m} \varepsilon_i N_i$$

Subtract

$$(\varepsilon_1 - \varepsilon_2) N_2 = \varepsilon_1 M - \varepsilon_1 \Sigma_{n=3}^{m} N_i - U + \Sigma_{n=3}^{m} \varepsilon_i N_i$$

$$= \varepsilon_1 M - U + \Sigma_{n=3}^{m} (\varepsilon_i - \varepsilon_1) N_i$$

so

$$N_2 = (\varepsilon_1 - \varepsilon_2)^{-1} [\, \varepsilon_1 M - U + \Sigma_{n=3}^{m} (\varepsilon_i - \varepsilon_1) N_i] = N_2(N_3, N_4 .... N_m)$$

Now do it the other way

$$\varepsilon_2 N_1 + \varepsilon_2 N_2 = \varepsilon_2 M - \varepsilon_2 \Sigma_{n=3}^{m} N_i$$
$$\varepsilon_1 N_1 + \varepsilon_2 N_2 = U - \Sigma_{n=3}^{m} \varepsilon_i N_i$$

Subtract bottom from top

$$(\varepsilon_2 - \varepsilon_1) N_1 = \varepsilon_2 M - \varepsilon_2 \Sigma_{n=3}^{m} N_i - U + \Sigma_{n=3}^{m} \varepsilon_i N_i$$

$$= \varepsilon_2 M - U + \Sigma_{n=3}^{m} (\varepsilon_i - \varepsilon_2) N_i$$

so then

$$N_1 = (\varepsilon_2 - \varepsilon_1)^{-1} [\, \varepsilon_2 M - U + \Sigma_{n=3}^{m} (\varepsilon_i - \varepsilon_2) N_i]$$

Now assume $\varepsilon_2 > \varepsilon_1$ just by convention. Then write

$$N_1 = + (\varepsilon_2 - \varepsilon_1)^{-1} [\, \varepsilon_2 M - U + \Sigma_{n=3}^{m} (\varepsilon_i - \varepsilon_2) N_i]$$
$$N_2 = - (\varepsilon_2 - \varepsilon_1)^{-1} [\, \varepsilon_1 M - U + \Sigma_{n=3}^{m} (\varepsilon_i - \varepsilon_1) N_i]$$

Notice that

$$\partial N_1 / \partial N_3 = + (\varepsilon_2 - \varepsilon_1)^{-1} [\, (\varepsilon_3 - \varepsilon_2) \,]$$
$$\partial N_2 / \partial N_3 = - (\varepsilon_2 - \varepsilon_1)^{-1} [\, (\varepsilon_3 - \varepsilon_1) \,]$$

and in general

$$\partial N_1 / \partial N_i = (\varepsilon_2 - \varepsilon_1)^{-1} [\, (\varepsilon_i - \varepsilon_2) \,] \qquad i = 3,4....m$$
$$\partial N_1 / \partial N_i = - (\varepsilon_2 - \varepsilon_1)^{-1} [\, (\varepsilon_i - \varepsilon_1) \,]$$

So this is the first time I have done this.

Now let F be some generic function of all the N_i. Then we have

$F(N_1(N_3 \ldots N_m), N_2(N_3 \ldots N_m), N_3, N_4 \ldots N_m)$

$$dF/dN_3 = \partial F/\partial N_1 \, \partial N_1/\partial N_3 + \partial F/\partial N_2 \, \partial N_2/\partial N_3 + \partial F/\partial N_3$$

$$= F_1 \quad (\varepsilon_2 - \varepsilon_1)^{-1} [\, (\varepsilon_3 - \varepsilon_2) \,] + F_2 \, (- \, (\varepsilon_2 - \varepsilon_1)^{-1} [\, (\varepsilon_3 - \varepsilon_1) \,]) + F_3$$

This certainly has an interesting form. Rewrite

$$dF/dN_3 = \frac{\varepsilon_3 - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} F_1 - \frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} F_2 + F_3$$

More generally,

$$dF/dN_i = \partial F/\partial N_1 \, \partial N_1/\partial N_i + \partial F/\partial N_2 \, \partial N_2/\partial N_i + \partial F/\partial N_i \qquad i = 3,4...m$$

so

$$dF/dN_i = \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} F_1 - \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} F_2 + F_i \qquad i = 3,4...m$$

and notice where the i's are located on the right side!

So, if you wanted to find the critical points of this unconstrained function $F(N_3,....N_m)$ you would set all these derivatives to 0

$$0 = \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} F_1 - \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} F_2 + F_i \qquad i = 3,4...m$$

Let's try an example. Suppose F =f

$$f = \Sigma_i [\, N_i \ln g_i \,] - \Sigma_i [\, \ln N_i! \,]$$

We then have these equations to solve for the max:

$$f_i = \ln(g_i/N_i) = \ln g_i - \ln N_i \qquad \text{// from above}$$

$$0 = \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} f_1 - \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} f_2 + f_i$$

or

$$0 = \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} \ln(g_1/N_1) - \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} \ln(g_2/N_2) + \ln(g_i/N_i) = 0 \qquad i = 3,4...m$$

But

$$N_1 = +(\varepsilon_2 - \varepsilon_1)^{-1}[\,\varepsilon_2 M - U + \Sigma_{n=3}^{m}(\varepsilon_i - \varepsilon_2)N_i]$$
$$N_2 = -(\varepsilon_2 - \varepsilon_1)^{-1}[\,\varepsilon_1 M - U + \Sigma_{n=3}^{m}(\varepsilon_i - \varepsilon_1)N_i]$$

Suppose we define

$$s_i \equiv \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} \qquad r_i \equiv \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1}$$

and then our equations are

$$0 = s_i \ln(g_1/N_1) - r_i \ln(g_2/N_2) + \ln(g_i/N_i) = 0 \qquad i = 3,4...m$$

or

$$0 = \ln(g_1/N_1)^{s_i} + \ln(g_2/N_2)^{-r_i} + \ln(g_i/N_i) = 0 \qquad i = 3,4...m$$

or

$$0 = \ln\left[\,(g_1/N_1)^{s_i}(g_2/N_2)^{-r_i}(g_i/N_i)\,\right] = 0 \qquad i = 3,4...m$$

But this says

$$(g_1/N_1)^{s_i}(g_2/N_2)^{-r_i}(g_i/N_i) = 1 \qquad i = 3,4...m$$

But these are very complicated equations because we have to use

$$N_1 = +(\varepsilon_2 - \varepsilon_1)^{-1}[\,\varepsilon_2 M - U + \Sigma_{n=3}^{m}(\varepsilon_i - \varepsilon_2)N_i]$$
$$N_2 = -(\varepsilon_2 - \varepsilon_1)^{-1}[\,\varepsilon_1 M - U + \Sigma_{n=3}^{m}(\varepsilon_i - \varepsilon_1)N_i]$$

So maybe this just shows how difficult this problem is to solve by this brute force method! So this thread leads nowhere useful.

Back to the idea of "moving off the peak"

Go back to

$$f = \Sigma_{i=1}^{m}[(1+\ln g_i)N_i - N_i \ln N_i] \qquad (6.2.3)$$

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

Suppose we are at some vector $\{N_i\}$ (not necessarily the peak) and we "move a little". What happens to f?

I already know that

$$N_1 + N_2 + N_3 + \Sigma_{n=4}^{m} N_i = M$$

$$\varepsilon_1 N_1 + \varepsilon_2 N_2 + \varepsilon_3 N_3 + \Sigma_{n=4}^{m} \varepsilon_i N_i = U$$

Suppose we concoct a "movement" such that only N_1, N_2 and N_3 change and all other N_i stay constant. Then one surely can write these 2 equations in 3 unknowns,

$$dN_1 + dN_2 + dN_3 = 0$$
$$\varepsilon_1 dN_1 + \varepsilon_2 dN_2 + \varepsilon_3 dN_3 = 0$$

Now do as was done above to solve for dN_2 and dN_3 both in terms of dN_1

$$\varepsilon_1 dN_1 + \varepsilon_1 dN_2 + \varepsilon_1 dN_3 = 0$$
$$\varepsilon_1 dN_1 + \varepsilon_2 dN_2 + \varepsilon_3 dN_3 = 0$$

Subtract

$$(\varepsilon_1 - \varepsilon_2) dN_2 + (\varepsilon_1 - \varepsilon_3) dN_3 = 0$$

Then we can replace

$$dN_3 = - \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 - \varepsilon_3} \, dN_2$$

and therefore

$$dN_1 + dN_2 + dN_3 = 0$$

$$dN_1 + dN_2 - \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 - \varepsilon_3} \, dN_2 = 0$$

$$dN_1 = dN_2 \left(\frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 - \varepsilon_3} - 1 \right) = dN_2 \left(\frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 - \varepsilon_3} - \frac{\varepsilon_1 - \varepsilon_3}{\varepsilon_1 - \varepsilon_3} \right) = dN_2 \, \frac{\varepsilon_3 - \varepsilon_2}{\varepsilon_1 - \varepsilon_3}$$

and this shows that

$$dN_2 = \frac{\varepsilon_1 - \varepsilon_3}{\varepsilon_3 - \varepsilon_2} \, dN_1$$

Then we know that

$$dN_3 = - \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 - \varepsilon_3} \, dN_2 = - \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 - \varepsilon_3} \, \frac{\varepsilon_1 - \varepsilon_3}{\varepsilon_3 - \varepsilon_2} \, dN_1 = \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} \, dN_1$$

Now assume that ε_1 is the lowest energy, so write with all positives

$$dN_2 = - \frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} dN_1$$

$$dN_3 = \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} dN_1$$

This says that if you make a free small movement dN_1, the other two variables have to change as shown

The first ratio is greater than 1, whereas the second could be < or > 1 depending on energy spacing, where again I assume ε_1 is lowest.

NOW consider:

$$f(N_1,N_2,N_3....N_m) = \Sigma_{i=1}^{m} [(1+\ln g_i)N_i - N_i \ln N_i] \qquad (6.2.3)$$

We are sitting at some general vector **N**. We now make a change $\{dN_1. dN_2, dN_3\}$ consistent with the rules above. What happens to F?

$$df = f_1 dN_1 + f_2 dN_2 + f_3 dN_3 \qquad \text{// true only for differentials}$$

$$= (\ln g_1 - \ln N_1) dN_1 + (\ln g_2 - \ln N_2) [- \frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} dN_1] + (\ln g_3 - \ln N_3) [\frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} dN_1]$$

$$= \{ (\ln g_1 - \ln N_1) + (\ln g_2 - \ln N_2) [- \frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2}] + (\ln g_3 - \ln N_3) [\frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2}] \} dN_1$$

$$= - \{ \ln(N_1/g_1) - \ln(N_2/g_2) \frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} + \ln(N_3/g_3) \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} \} dN_1$$

Notice how i = 4,5...m don't enter into this "movement" d**N** where only 1,2,3 move.

If our vector **N** is in some arbitrary location, there is some df as above. But if **N** is the solution vector, then we know that

$$\ln(N_i/g_i) = \lambda_1 + \lambda_2 \varepsilon_i = \lambda_1 - \beta \varepsilon_i \qquad (6.2.9)$$

So if we start with the solution vector N we find that

$$df = - \{ (\lambda_1 - \beta\varepsilon_1) - (\lambda_1 - \beta\varepsilon_2) \frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} + (\lambda_1 - \beta\varepsilon_3) \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} \} dN_1$$

$$= - \{ \lambda_1 [1 - \frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} + \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2}] - \beta [\varepsilon_1 - \varepsilon_2 \frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} + \varepsilon_3 \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2}] \} dN_1$$

$$= - \{ \lambda_1 [\frac{\varepsilon_3 - \varepsilon_2}{\varepsilon_3 - \varepsilon_2} - \frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} + \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2}] - \beta [\varepsilon_1 \frac{\varepsilon_3 - \varepsilon_2}{\varepsilon_3 - \varepsilon_2} - \varepsilon_2 \frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} + \varepsilon_3 \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2}] \} dN_1$$

$= - \{ \lambda_1 [0] - \beta [0] \} dN_1$

$= 0$

This is the expected answer because we are at a critical point. So this more or less validates what I am doing here.

Let's now try for the curvature!!

Start as above to get the first derivative

Now let F be some generic function of all the N_i. Then we have

$F(N_1(N_3 \ldots N_m), N_2(N_3 \ldots N_m), N_3, N_4 \ldots N_m)$

$dF/dN_3 = \partial F/\partial N_1 \, \partial N_1/\partial N_3 + \partial F/\partial N_2 \, \partial N_2/\partial N_3 + \partial F/\partial N_3$

$= F_1 \ (\varepsilon_2 - \varepsilon_1)^{-1} [(\varepsilon_3 - \varepsilon_2)] + F_2 (- (\varepsilon_2 - \varepsilon_1)^{-1} [(\varepsilon_3 - \varepsilon_1)]) + F_3$

This certainly has an interesting form. Rewrite

$$dF/dN_3 = \frac{\varepsilon_3 - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} F_1 - \frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} F_2 + F_3$$

More generally,

$dF/dN_i = \partial F/\partial N_1 \, \partial N_1/\partial N_i + \partial F/\partial N_2 \, \partial N_2/\partial N_i + \partial F/\partial N_i \qquad i = 3,4 \ldots m$

so

$$dF/dN_i = \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} F_1 - \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} F_2 + F_i \qquad i = 3,4 \ldots m$$

Now consider

$$dF_1/dN_i = \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} F_{11} - \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} F_{12} + F_{1i}$$ F_{ij} are all second partials!

$$dF_2/dN_i = \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} F_{21} - \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} F_{22} + F_{2i}$$ F_{ij} are all second partials

$$dF_i/dN_i = \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} F_{i1} - \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} F_{i2} + F_{ii}$$ no sum on i of course

Then I get

$$d^2F/dN_i^2 = \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1}\left[\frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} F_{11} - \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} F_{12} + F_{1i}\right]$$

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

$$+ \left[\frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} F_{i1} - \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} F_{i2} + F_{ii}\right] \qquad i = 3,4....M$$

Now at once apply this to F = f where we know that

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

$$f_{ij} = \partial f_i/\partial N_j = -\delta_{ij}\,(1/N_i)$$

We then write (since i = 3,4....m)

$$d^2f/dN_i^2 = \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1}\left[\frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} f_{11}\right]$$

$$- \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1}\left[-\frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} f_{22}\right]$$

$$+ [+ f_{ii}]$$

$$= \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1}\frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1} f_{11} + \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1}\frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1} f_{22} + f_{ii}$$

$$= \frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1}\frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1}(-1/N_1) + \frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1}\frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1}(-1/N_2) + (-1/N_i)$$

$$= -\left\{\left[\frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1}\right]^2 \frac{1}{N_1} + \left[\frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1}\right]^2 \frac{1}{N_2} + \frac{1}{N_i}\right\} \qquad i = 3,4....m$$

Amazingly this comes out definitely negative, meaning cupping down, which is correct. This is a first!

Here is the conclusion:

$$d^2f/dN_i^2 = -\left\{\left[\frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1}\right]^2 \frac{1}{N_1} + \left[\frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1}\right]^2 \frac{1}{N_2} + \frac{1}{N_i}\right\} \qquad i = 3,4....m$$

for any vector **N**, not just the solution vector. In general, I would say

$d^2f/dN_i^2 \sim -(1/N_k)$ where N_k is one of the vectors , just order of

Now consider our earlier calculation where NOW I am taking about FULL derivatives, so be very careful with notation!!

$\Omega = e^f$

$\Omega_i = \Omega f_i$

$\Omega_{ii} = \Omega f_{ii} + \Omega_i f_i = \Omega f_{ii} + \Omega f_i^2 = \Omega (f_{ii} + f_i^2)$ i = 3,4...m

which really means

$(d^2\Omega/dN_i^2) = \Omega [(d^2f/dN_i^2) + (df/dN_i)^2]$

Now at the peak, we know $(df/dN_i) = 0$ and we even showed it above. so therefore

$$(d^2\Omega/dN_i^2) = -\Omega \{ [\frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1}]^2 \frac{1}{N_1} + [\frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1}]^2 \frac{1}{N_2} + \frac{1}{N_i} \} \quad i = 3,4....m$$

and this is a very major result!!

(1) it is negative so peak is really a maximum

(2) it is a very large number because although $1/N_i$ is small, Ω is extremely large!

In our example, the above would read (N_3 is the only other N_i)

$$(d^2\Omega/dN_3^2) = -\Omega \{ [\frac{\varepsilon_3 - \varepsilon_2}{\varepsilon_2 - \varepsilon_1}]^2 \frac{1}{N_1} + [\frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_2 - \varepsilon_1}]^2 \frac{1}{N_2} + \frac{1}{N_3} \}$$

$$= -\Omega \{ \frac{1}{N_1} + 4 \frac{1}{N_2} + \frac{1}{N_3} \} \approx -\Omega \{ 6/333 \} = \text{very large}$$

so the corresponding curvature radius at the peak would be very small.

So exactly how large is Ω at the peak?

$$f = \Sigma_{i=1}^m [(1+\ln g_i)N_i - N_i \ln N_i] \qquad (6.2.3)$$

$$N_i = g_i e^{\lambda_1} e^{\lambda_2 \varepsilon_i} . \qquad (6.2.9)$$

So write

$N_i = A g_i e^{-\beta \varepsilon_i}$

Then we have

$$f = \Sigma_{i=1}^{m} [(1+\ln g_i)N_i - N_i \ln N_i \,] \;=\; \Sigma_i \, N_i \, [\, (1+\ln g_i) - \ln N_i \,]$$

$$= \Sigma_{i=1}^{m} [(1+\ln g_i)(A\, g_i\, e^{-\beta \varepsilon_i}) - (A\, g_i\, e^{-\beta \varepsilon_i}) \ln(A\, g_i\, e^{-\beta \varepsilon_i}) \,]$$

$$\approx \; \Sigma_i \, [\ln g_i(A\, g_i\, e^{-\beta \varepsilon_i}) - (A\, g_i\, e^{-\beta \varepsilon_i}) (\ln A + \ln g_i - \beta\, \varepsilon_i) \,]$$

$$= \;\; \Sigma_i \, (A\, g_i\, e^{-\beta \varepsilon_i}) \, [\ln g_i - \; (\ln A + \ln g_i - \beta\, \varepsilon_i) \,]$$

$$= \;\; \Sigma_i \, (A\, g_i\, e^{-\beta \varepsilon_i}) \, [\ln g_i - \; \ln A - \ln g_i + \beta\, \varepsilon_i \,]$$

$$= \;\; \Sigma_i \, (A\, g_i\, e^{-\beta \varepsilon_i}) \, [- \; \ln A + \beta\, \varepsilon_i \,]$$

$$= \;\; \Sigma_i \, N_i \, [- \; \ln A + \beta\, \varepsilon_i \,]$$

$$= \; -\ln(A)\, M + \beta\, U$$

where

$$A = \frac{M}{\Sigma_i g_i \, e^{-\beta \varepsilon_i}} \;. \qquad (6.2.14)$$

But from just the first line I know that

$$f \;\approx\; \Sigma_i \, N_i \, \ln(g_i/N_i) \; + \Sigma_i \, N_i$$

Now suppose we just assume that $\ln(g_i/N_i) = \ln(5000/333) = 2.71$. Then

$$f_1 \approx 2.709\, M \;=\; 2.709 * 1000 = 2709$$

$$f_2 \approx \; M = 1000$$

$$f \;= f_1 + f_2 = 2709 + 1000 \;= 3709$$

Then

$$\Omega = e^{f} = e^{3709} \;\approx\; (1/2) * 10^{1611} \qquad \text{//Maple}$$

The Maple plot shows directly that the peak value is $250{,}000 * 10^{1600} \;= 2.5 * 10^{1605}$

So why am I off by something like 100,000 ??? Probably Sterling. Correct formula is

$$f = \ln\Omega \;=\; \Sigma_i \, [\, N_i \, \ln g_i \,] \; - \Sigma_i \, [\, \ln N_i! \,]$$

In my test case we have $N_i = 333$ and so

$f = \Sigma_i [N_i \ln(5000)] - \Sigma_i [\ln N_i!]$

$= 1000*\ln(5000) - 3*\ln[(1000/3)!]$

$= 8517 - 4820 = 3697$

$\Omega = e^f = e^{3697} = 0.4 * 10^{1606}$

OK, so now I know how large Ω is at least in my example.

Now go back to curvature

$$(d^2\Omega/dN_i^2) = -\Omega \{ [\frac{\varepsilon_i - \varepsilon_2}{\varepsilon_2 - \varepsilon_1}]^2 \frac{1}{N_1} + [\frac{\varepsilon_i - \varepsilon_1}{\varepsilon_2 - \varepsilon_1}]^2 \frac{1}{N_2} + \frac{1}{N_i} \} \quad i = 3,4....m$$

What is Ω for a more real-world example? Suppose we just assume that $g_i = 10^7 N_i$ as a ballpark number. And maybe $N_i = 10^{20}$ as a ballpark number for a small amount of gas. Then

$$\frac{g_1^{N_1}}{N_1!} \approx (10^7 N_1)$$

well not sure this helps anyone. I think best to stick to the example.

I notice from my plot that the curvature at the peak made into a semicircle does NOT give a good estimate for the width of the peak. So, again sticking with the same, I have

$$\Omega(N_1,N_2,N_3) = \frac{g_1^{N_1}}{N_1!} \frac{g_2^{N_2}}{N_2!} \frac{g_3^{N_3}}{N_3!}$$

$N_2 = -2N_1 - U + 3M = -2N_1 + M$ $\qquad$ $U = 2M$ for ∞ temp

$N_3 = N_1 - 2M + U = N_1$

So there you have it

$$\Omega(N_1) \equiv \Omega(N_1,N_2(N_1),N_3(N_1)) = \frac{g_1^{N_1}}{N_1!} \frac{g_2^{M-2N_1}}{(M-2N_1)!} \frac{g_3^{N_1}}{N_1!}$$

$$= \frac{g^M}{(N_1)!(N_1)!(M-2N_1)!}$$

I plotted this with g = 5000, M = 1000 as in example and the plot comes out what I expect.

Now, where is the half-height of such a plot?? I guess the g^M factor cancels and we can write

$$1/2 = \Omega_{half}(N_1)\Omega(peak) = [(N_1)!(N_1)!(M-2N_1)!] / [(333)!(333)!(333)!]$$

So you have to solve

$$[(333)!]^3 (1/2) = [(N_1)!]^2 (1000-2N_1)!]$$

What a pain! Let's try it in terms of f instead.

$$f = \Sigma_{i=1}^{m} [(1+\ln g_i)N_i - N_i \ln N_i] \qquad (6.2.3)$$

$$= \Sigma_{i=1}^{m} N_i[(1+\ln g_i) - \ln N_i]$$

If the g_i are the same this says

$$f = (1+\ln g) M - \Sigma_{i=1}^{m} N_i \ln N_i$$

$$= (1+\ln g) M - 2 N_1 \ln N_1 - (M-2N_1)\ln (M-2N_1)$$

and the plot looks right! So consider

$$\Omega_h/\Omega_p = 1/2 \quad \Rightarrow f_h - f_p = \ln(1/2) = - \ln(2)$$

$$= \quad f_p - f_h = \ln(2) = 0.7$$

So f drops about 1 single unit. Let's write the equation

$$f_p = (1+\ln g) M - 2 N_{1p} \ln N_{1p} - (M-2N_{1p})\ln (M-2N_{1p})$$

$$f_h = (1+\ln g) M - 2 N_{1h} \ln N_{1h} - (M-2N_{1h})\ln (M-2N_{1h})$$

$$f_p - f_h = - 2 N_{1p} \ln N_{1p} - (M-2N_{1p})\ln (M-2N_{1p}) - [- 2 N_{1h} \ln N_{1h} - (M-2N_{1h})\ln (M-2N_{1h})]$$

$$= - 2 N_{1p} \ln N_{1p} - (M-2N_{1p})\ln (M-2N_{1p}) + 2 N_{1h} \ln N_{1h} + (M-2N_{1h})\ln (M-2N_{1h})]$$

$$= -(667)\ln(333) - (333) \ln(333) + 2 N_{1h} \ln N_{1h} + (M-2N_{1h})\ln (M-2N_{1h})] = 0.7$$

Again I see no intuitive solution! Suppose I assume the log terms are the same for half and peak. Then

$$-(667)\ln(333) - (333) \ln(333) + 2 N_{1h} \ln(333) + (M-2N_{1h})\ln (333)] = 0.7$$

$$[-667 - 333 + 2N_{1h} + (1000 - 2N_{1h}\} \ln(333) = 0.7 \qquad \text{// answer is lost!}$$

OK, write $N_h = N_p + d$ d is very small

$$\ln N_{1h} = \ln(N_{1p} + d) = \ln[(N_{1p})(1 + d/N_{1p})] = \ln N_{1p} \ln(1 + d/N_{1p}) \approx \ln N_{1p} * (d/N_{1p})$$

$$\ln (M-2N_{1h}) = \ln (M-2N_{1p} - 2d) = \ln(M-2N_{1p})* [-2d/(M-2N_{1p})]$$

Then

$$f_p - f_h = - 2 N_{1p}\ln N_{1p} - (M-2N_{1p})\ln (M-2N_{1p}) - [- 2 N_{1h}\ln N_{1h} - (M-2N_{1h})\ln (M-2N_{1h})]$$

$$= - 2 N_{1p}\ln N_{1p} - (M-2N_{1p})\ln (M-2N_{1p}) + 2N_{1h}\ln N_{1h} + (M-2N_{1h})\ln (M-2N_{1h})$$

$$\approx - 2 N_{1p}\ln N_{1p} - (M-2N_{1p})\ln (M-2N_{1p})$$

STOP (maybe later). Go back to the curvature of f:

$$d^2f/dN_3^2 = - \{ [\frac{\varepsilon_3 - \varepsilon_2}{\varepsilon_2 - \varepsilon_1}]^2 \frac{1}{N_1} + [\frac{\varepsilon_3 - \varepsilon_1}{\varepsilon_2 - \varepsilon_1}]^2 \frac{1}{N_2} + \frac{1}{N_3} \} \qquad i = 3,4....m$$

$$= - \{ \frac{1}{N_1} + 4 \frac{1}{N_2} + \frac{1}{N_3} \} = - 6/333.$$

Very good. Now write

$$f(N_{1p} + d) = f(N_{1p}) + (1/2) f'' (d)^2$$

or

$$f_h = f_p + 1/2 * d^2 * [-6/333]$$

or

$$f_h = f_p - (3/333)d^2$$

or

$$f_p - f_h = 0.7 = d^2/111 \qquad => \qquad d^2 = 111*.7 = 78 \quad = \text{expected half distance away from peak}$$

$$d = 9$$

so the full half width is then about 18. And this looks VERY good!

For general M and our simple model problem, we get N = M/3 and so

$$f'' = - 6/N = -18/M$$

$$f_h = f_p + (1/2) d^2 [-18/M]$$

$$f_p - f_h = (1/2) d^2 [18/M] = 0.7$$

$0.7 = (9/M)d^2$ $\quad d^2 = 0.7\ M/9 = .078\ M$ $\quad d = .28\sqrt{M}$

half width of bell = $.56\sqrt{M}$

as a percentage $\quad \Delta N/N = .56\sqrt{M} / [M/3] = .56*3 /\sqrt{M} = 1.68/\sqrt{M}$

So if M = 1000 this says

$\Delta N/N = .053$ $\quad$ check: $\quad 18/333 = .054$

So if $M = 10^{20}$ then $\Delta N/N = 1.68/ 10^{10} = 1.68 \times 10^{-10}$ $\quad$ very narrow peak!~