A Derivation of local energy

Beginning from the definition of the local energy as defined by eq. (10) we get

$$E_L = \frac{1}{\Psi}\hat{H}\Psi = \frac{1}{\Psi}\sum_{i=1}^{N_P}\left(-\frac{1}{2}\nabla_i^2 + \frac{1}{2}\omega^2 r_i^2\right)\Psi + \frac{1}{\Psi}\sum_{i<j}\frac{1}{r_{ij}}\Psi,$$

we note that the wave-function factors cancel for all terms except for the term containing the differential operator. We thus get

$$E_L = \sum_{i=1}^{N_P}\left(-\frac{1}{2}\frac{1}{\Psi}\nabla_i^2\Psi + \frac{1}{2}\omega^2 r_i^2\right) + \sum_{i<j}\frac{1}{r_{ij}}.$$

Hence, the only non-trivial term is the kinetic term, using the relation

$$\frac{1}{\Psi}\nabla^2\Psi = \nabla^2 \ln\Psi + (\vec{\nabla}\ln\Psi)^2,$$

we get an expression for the local energy as

$$E_L = \sum_{i=1}^{N_P}\left(-\frac{1}{2}\nabla_i^2\ln\Psi - \frac{1}{2}(\vec{\nabla}_i\ln\Psi)^2 + \frac{1}{2}\omega^2 r_i^2\right) + \sum_{i<j}\frac{1}{r_{ij}}.$$

Thus we only need to find the expressions of $\nabla^2\ln\Psi$ and $\vec{\nabla}\ln\Psi$. As

$$\vec{\nabla}\ln\Psi = \sum_k \frac{\partial}{\partial x_k}\ln\Psi\hat{e}_k, \quad \nabla^2\ln\Psi = \sum_k\frac{\partial^2}{\partial x_k^2}\ln\Psi,$$

the problem further reduces to finding $\frac{\partial}{\partial x_k}\ln\Psi$ and $\frac{\partial^2}{\partial x_k^2}\ln\Psi$ for fixed k.

As

$$\ln\Psi = -\ln Z - \sum_{i=1}^{M}\frac{(x_i-a_i)^2}{2} + \sum_{j=1}^{N}\ln\left(1+e^{b_j+\sum_{i=1}^M x_i w_{ij}}\right),$$

it follows that

$$\begin{aligned}\frac{\partial}{\partial x_k}\ln\Psi &= \frac{\partial}{\partial x_k}\left(-\sum_{i=1}^{M}\frac{(x_i-a_i)^2}{2} + \sum_{j=1}^{N}\ln\left(1+e^{b_j+\sum_{i=1}^M x_i w_{ij}}\right)\right)\\ &= -(x_k-a_k) + \sum_{j=1}^{N}\frac{w_{kj}}{1+e^{-b_j-\sum_{i=1}^M x_i w_{ij}}}.\end{aligned}$$

As for the second derivative

$$\frac{\partial^2}{\partial x_k^2}\ln\Psi = \frac{\partial}{\partial x_k}\ln\Psi\left(-(x_k-a_k) + \sum_{j=1}^{N}\frac{w_{kj}}{1+e^{-b_j-\sum_{i=1}^M x_i w_{ij}}}\right)$$

$$= -1 + \sum_{j=1}^{N} w_{kj}\frac{\partial}{\partial x_k}\left(1+e^{-b_j-\sum_{j=1}^M x_i w_{ij}}\right)^{-1} = -1 + \sum_{j=1}^{N}\frac{w_{kj}^2 e^{b_j+\sum_{i=1}^M x_i w_{ij}}}{\left(1+e^{b_j+\sum_{i=1}^M x_i w_{ij}}\right)^2}.$$

From this we conclude that the local energy is of the form

$$E_L = \sum_{i=1}^{N_P}\left(-\frac{1}{2}\nabla^2\ln\Psi - \frac{1}{2}(\vec{\nabla}\ln\Psi)^2 + \frac{1}{2}\omega^2 r_i^2\right) + \sum_{i<j}\frac{1}{r_{ij}}, \tag{25}$$

with

$$\frac{\partial}{\partial x_k}\ln\Psi = -(x_k-a_k) + \sum_{j=1}^{N}\frac{w_{kj}}{1+e^{-b_j-\sum_{i=1}^M x_i w_{ij}}}, \tag{26}$$

and

$$\frac{\partial^2}{\partial x_k^2}\ln\Psi = -1 + \sum_{j=1}^{N}\frac{w_{kj}^2 e^{b_j+\sum_{i=1}^M x_i w_{ij}}}{\left(1+e^{b_j+\sum_{i=1}^M x_i w_{ij}}\right)^2}. \tag{27}$$

B Variational parameter derivatives

Again, starting from

$$\ln \Psi = -\ln Z - \sum_{i=1}^{M} \frac{(x_i - a_i)^2}{2} + \sum_{j=1}^{N} \ln \left(1 + e^{b_j + \sum_{i=1}^{M} x_i w_{ij}}\right),$$

one can almost read off the derivative of $\ln \Psi$ w.r.t a_i and b_i. The derivatives are then,

$$\frac{\partial}{\partial a_m} \ln \Psi = x_m - a_m.$$

$$\frac{\partial}{\partial b_m} \ln \Psi = \frac{\partial}{\partial b_m} \sum_{j=1}^{N} \ln \left(1 + e^{b_j + \sum_{i=1}^{M} x_i w_{ij}}\right) = \frac{1}{1 + e^{-b_m - \sum_{i=1}^{M} x_i w_{im}}}.$$

$$\begin{aligned}\frac{\partial}{\partial w_{nm}} \ln \Psi &= \frac{\partial}{\partial w_{nm}} \sum_{j=1}^{N} \ln \left(1 + e^{b_j + \sum_{i=1}^{M} x_i w_{ij}}\right) = \sum_{i,l}^{M,N} \frac{x_l e^{b_j + \sum_{i=1}^{M} x_i w_{ij}}}{1 + e^{b_j + \sum_{i=1}^{M} x_i w_{ij}}} \delta_{nl} \delta_{mj} \\ &= \frac{x_n}{1 + e^{-b_m - \sum_{i=1}^{M} x_i w_{im}}}.\end{aligned}$$

Gathering the results, we see that the derivatives are

$$\frac{\partial}{\partial a_m} \ln \Psi = x_m - a_m, \tag{28}$$

$$\frac{\partial}{\partial b_m} \ln \Psi = \frac{1}{1 + e^{-b_m - \sum_{i=1}^{M} x_i w_{im}}}, \tag{29}$$

$$\frac{\partial}{\partial w_{nm}} \ln \Psi = \frac{x_n}{1 + e^{-b_m - \sum_{i=1}^{M} x_i w_{im}}}. \tag{30}$$

C Marginal probability distribution

One can find the marginal probability distribution for x by summing over the set of all possible micro-states $\{h = 0, 1\}$. The expression is derived as

$$\begin{aligned}p(x) &= \frac{1}{Z} \sum_{\{h\}} e^{-H(x,h)} = \frac{1}{Z} \sum_{\{h\}} e^{-\sum_{i=1}^{M} \frac{(x_i - a_i)^2}{2} + \sum_{j=1}^{N} b_j h_j + \sum_{i,j}^{M,N} x_i w_{ij} h_j} \\ &= \frac{1}{Z} e^{-\sum_{i=1}^{M} \frac{(x_i - a_i)^2}{2}} \sum_{\{h\}} e^{\sum_{j=1}^{N} b_j h_j + \sum_{i,j}^{M,N} x_i w_{ij} h_j}.\end{aligned}$$

Evaluating the sum over all different ensembles we get

$$\begin{aligned}\sum_{\{h\}} e^{\sum_{j=1}^{N} b_j h_j + \sum_{i,j}^{M,N} x_i w_{ij} h_j} &= \sum_{\{h_1=0,1\}} e^{b_1 h_1 + \sum_{i}^{M} x_i w_{i1} h_1} \sum_{\{h_2=0,1\}} e^{b_2 h_2 + \sum_{i}^{M} x_i w_{i2} h_2} \dots \sum_{\{h_N=0,1\}} e^{b_N h_N + \sum_{i}^{M} x_i w_{iN} h_N} \\ &= \left(1 + e^{b_1 + \sum_{i}^{M} x_i w_{i1}}\right) \left(1 + e^{b_2 + \sum_{i}^{M} x_i w_{i2}}\right) \dots \left(1 + e^{b_N + \sum_{i}^{M} x_i w_{iN}}\right) \\ &= \prod_{j=1}^{N} (1 + e^{b_j + \sum_{i}^{M} x_i w_{ij}}).\end{aligned}$$

Thus with this last result at hand, the expression for the marginal probability becomes

$$p(x) = \frac{1}{Z} e^{-\sum_{i}^{M} (x_i - a_i)^2} \prod_{k}^{N} (1 + e^{b_k + \sum_{j}^{M} x_j w_{jk}}). \tag{31}$$