Notation:

- visible nodes $\vec{x} \in \mathbb{R}^M$ - gaussian units (position coordinates)
- hidden nodes $\vec{h} \in \mathbb{R}^N$ - binary units
- visible biases $\vec{a} \in \mathbb{R}^M$
- hidden biases $\vec{b} \in \mathbb{R}^N$
- interaction weights $\hat{W} \in \mathbb{R}^{M \times N}$
- jth column vector of weight matrix $\vec{W}_j \in \mathbb{R}^M$
- ith row vector of weight matrix $\vec{W}_i^T \in \mathbb{R}^N$
- variational parameters $\vec{\theta} = (a_0, \cdots, a_{M-1}, b_0, \cdots, b_{N-1}, W_{0,0}, \cdots, W_{M-1,N-1})$

"Energy" of a configuration of nodes:

$$
\begin{aligned}
E(\vec{x}, \vec{h}) &= \frac{1}{2\sigma^2} \sum_{i=0}^{M-1} (x_i - a_i)^2 - \sum_{j=0}^{N-1} b_j h_j - \frac{1}{\sigma^2} \sum_{i=0}^{M-1} \sum_{j=0}^{N-1} x_i W_{ij} h_j \\
&= \frac{1}{2\sigma^2} \|\vec{x} - \vec{a}\|^2 - \vec{b}^T \vec{h} - \frac{1}{\sigma^2} \vec{x}^T \hat{W} \vec{h}
\end{aligned}
$$

Use the marginal probability to represent the wavefunction as a function of the RBM inputs:

$$
\begin{aligned}
\Psi_{NQS}(\vec{x}) &= \frac{1}{Z} \sum_{\vec{h}} e^{-E(\vec{x}, \vec{h})} \\
&= \frac{1}{Z} \sum_{\vec{h}} \exp\left(-\frac{1}{2\sigma^2} \|\vec{x} - \vec{a}\|^2 + \vec{b}^T \vec{h} + \frac{1}{\sigma^2} \vec{x}^T \hat{W} \vec{h} \right) \\
&= \frac{1}{Z} \exp\left(-\frac{1}{2\sigma^2} \|\vec{x} - \vec{a}\|^2 \right) \sum_{\{h_j\}} \exp\left(\sum_{j=0}^{N-1} b_j h_j + \frac{1}{\sigma^2} \sum_{i=0}^{M-1} \sum_{j=0}^{N-1} x_i W_{ij} h_j \right) \\
&= \frac{1}{Z} \exp\left(-\frac{1}{2\sigma^2} \|\vec{x} - \vec{a}\|^2 \right) \prod_{j=0}^{N-1} \sum_{h_j=0}^{1} \exp\left(b_j h_j + \frac{1}{\sigma^2} \sum_{i=0}^{M-1} x_i W_{ij} h_j \right) \\
&= \frac{1}{Z} \exp\left(-\frac{1}{2\sigma^2} \|\vec{x} - \vec{a}\|^2 \right) \prod_{j=0}^{N-1} \left(1 + \exp\left(b_j + \frac{1}{\sigma^2} \vec{x}^T \vec{W}_j \right) \right)
\end{aligned}
$$

Hamiltonian for P D-dimensional particles in a harmonic oscillator ($\hbar = m = 1$) is

$$
\hat{H} = \frac{1}{2} \sum_{p=0}^{P-1} \left(-\nabla_p^2 + \sum_{d=0}^{D-1} \omega_d^2 r_{p,d}^2 \right) + \sum_{p<q} V_{int}(r_{pq}), \quad r_{pq} = \sqrt{\sum_{d=0}^{D-1} (r_{p,d} - r_{q,d})^2},
$$

where ∇_p^2 is the Laplacian with respect to the coordinates of the pth particle

$$\nabla_p = \sum_{d=0}^{D-1} \hat{n}_d \frac{\partial}{\partial r_{p,d}},$$
$$\nabla_p^2 = \nabla_p \cdot \nabla_p = \sum_{d=0}^{D-1} \frac{\partial^2}{\partial r_{p,d}^2},$$

and $\hat{n_d}$, $d = 0, ..., D-1$, denote the elementary unit vectors in each of the D dimensions.

We need to vectorize the coordinates of all the particles to input into the RBM:

$$\vec{x} = (r_{0,0}, \cdots, r_{0,D-1}, \cdots, r_{P-1,0}, \cdots, r_{P-1,D-1}) \in \mathbb{R}^M, \ \ M = PD$$

The visible biases and the rows of the weight matrix are organized in the same way. The mapping between coordinates and the visible nodes is:

$$r_{p,d} = x_{Dp+d}$$
$$x_i = r_{\text{floor}(i/D), i \text{mod} D}$$

Now we can write our representation of the wavefunction as a function of all coordinates:

$$\begin{aligned}
\Psi_{NQS}(\vec{R}) &= \frac{1}{Z} \exp\left(-\frac{1}{2\sigma^2} \sum_{p=0}^{P-1}\sum_{d=0}^{D-1} (r_{p,d} - a_{Dp+d})^2\right) \prod_{j=0}^{N-1} \left(1 + \exp\left(b_j + \frac{1}{\sigma^2} \sum_{p=0}^{P-1}\sum_{d=0}^{D-1} r_{p,d} W_{Dp+d,j}\right)\right) \\
&= \frac{1}{Z} \exp(A(\vec{R})) \prod_{j=0}^{N-1} \exp\left(\ln\left(1 + \exp\left(b_j + \frac{1}{\sigma^2} \sum_{p=0}^{P-1}\sum_{d=0}^{D-1} r_{p,d} W_{Dp+d,j}\right)\right)\right) \\
&= \frac{1}{Z} \exp(A(\vec{R})) \exp\left(\sum_{j=0}^{N-1} \ln\left(1 + \exp\left(b_j + \frac{1}{\sigma^2} \sum_{p=0}^{P-1}\sum_{d=0}^{D-1} r_{p,d} W_{Dp+d,j}\right)\right)\right) \\
&= \frac{1}{Z} \exp\left(A(\vec{R}) + B(\vec{R})\right)
\end{aligned}$$

$$\begin{aligned}
A(\vec{R}) &\equiv -\frac{1}{2\sigma^2} \sum_{p=0}^{P-1}\sum_{d=0}^{D-1} (r_{p,d} - a_{Dp+d})^2 = -\frac{1}{2\sigma^2} \sum_{i=0}^{M-1} (x_i - a_i)^2 = -\frac{1}{2\sigma^2} \|\vec{x} - \vec{a}\|^2 \\
B(\vec{R}) &\equiv \sum_{j=0}^{N-1} \ln\left(1 + \exp\left(B_j(\vec{R})\right)\right) \\
B_j(\vec{R}) &\equiv b_j + \frac{1}{\sigma^2} \sum_{p=0}^{P-1}\sum_{d=0}^{D-1} r_{p,d} W_{Dp+d,j} = b_j + \sum_{i=0}^{M-1} x_i W_{i,j} = b_j + \frac{1}{\sigma^2} \vec{x} \cdot \vec{W}_j
\end{aligned}$$

If the particles are low-density bosons with a hard-core interaction:

$$V_{int}(r_{pq}) = \begin{cases} \infty, & r_{pq} \leq a, \\ 0, & r_{pq} > a, \end{cases}$$

and if the particles are electrons ($e = 1$, $S = 0$) with the Coulomb interaction:

$$V_{int}(r_{pq}) = \frac{1}{r_{pq}}$$

The behaviors due to these interactions are accounted for in the trial wavefunction by a corresponding Jastrow factor so that the full trial wavefunction is

$$\Psi_T(\vec{R}) = \Psi_{NQS}(\vec{R})\exp(J(\vec{R})) = \frac{1}{Z}\exp\Big(A(\vec{R}) + B(\vec{R}) + J(\vec{R})\Big)$$

For bosons:

$$J_B(\vec{R}) = \sum_{p<q}\ln\left(1 - \frac{a}{r_{pq}}\right)$$

For electrons:

$$J_C(\vec{R}) = \sum_{p<q} r_{pq}$$

The local energy is defined as

$$E_L = \frac{1}{\Psi_T}\hat{H}\Psi_T$$

We want an analytical expression for the local energy in terms of our variational parameters $\vec{\theta}$. First, we have that

$$\frac{1}{\Psi_T}\nabla_p\Psi_T = \nabla_p A + \nabla_p B + \nabla_p J$$

$$\frac{1}{\Psi_T}\nabla_p^2\Psi_T = \nabla_p^2 A + \nabla_p^2 B + \nabla_p^2 J + \Big(\nabla_p A + \nabla_p B + \nabla_p J\Big)^2$$

Derivatives of A:

$$\begin{aligned}
A(\vec{R}) &\equiv -\frac{1}{2\sigma^2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1}(r_{p,d} - a_{Dp+d})^2, \\
\nabla_p A &= -\frac{1}{2\sigma^2}\sum_{d=0}^{D-1}\hat{n_d}\frac{\partial}{\partial r_{k,d}}\left\{\sum_{p'=0}^{P-1}\sum_{d'=0}^{D-1}(r_{p',d'} - a_{Dp'+d'})^2\right\} \\
&= -\frac{1}{2\sigma^2}\sum_{d=0}^{D-1}\sum_{p'=0}^{P-1}\sum_{d'=0}^{D-1}2(r_{p',d'} - a_{Dp'+d'})\delta_{p',p}\delta_{d',d}\hat{n_d} = \frac{1}{\sigma^2}\sum_{d=0}^{D-1}(a_{Dp+d} - r_{p,d})\hat{n_d} \\
\nabla_p^2 A &= \frac{1}{\sigma^2}\sum_{d=0}^{D-1}\hat{n}_d\frac{\partial}{\partial r_{p,d}}\cdot\sum_{d'=0}^{D-1}(a_{Dp+d'} - r_{p,d'})\hat{n_{d'}} = \frac{1}{\sigma^2}\sum_{d=0}^{D-1}\sum_{d'=0}^{D-1}(-1)\delta_{d',d} = -\frac{D}{\sigma^2}
\end{aligned}$$

Derivatives of B_j:

$$
\begin{aligned}
B_j(\vec{R}) &\equiv b_j + \frac{1}{\sigma^2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1} r_{p,d} W_{Dp+d,j} \\
\nabla_p B_j &= \sum_{d=0}^{D-1} \hat{n}_d \frac{\partial}{\partial r_{p,d}} \left\{ b_j + \frac{1}{\sigma^2}\sum_{p'=0}^{P-1}\sum_{d'=0}^{D-1} r_{p',d'} W_{Dp'+d',j} \right\} \\
&= \frac{1}{\sigma^2}\sum_{d=0}^{D-1}\sum_{p'=0}^{P-1}\sum_{d'=0}^{D-1} W_{Dp'+d',j}\delta_{p',p}\delta_{d',d}\hat{n}_d = \frac{1}{\sigma^2}\sum_{d=0}^{D-1} W_{Dp+d,j}\hat{n}_d \\
\nabla_p^2 B_j &= 0
\end{aligned}
$$

Derivatives of B:

$$
\begin{aligned}
B(\vec{R}) &\equiv \sum_{j=0}^{N-1} \ln\Big(1+\exp\big(B_j(\vec{R})\big)\Big) \\
\nabla_p B &= \sum_{j=0}^{N-1} \nabla_p \Big\{ \ln\Big(1+\exp\big(B_j\big)\Big)\Big\} = \sum_{j=0}^{N-1} \frac{1}{1+\exp(B_j)} \nabla_p \Big\{ 1+\exp\big(B_j\big)\Big\} \\
&= \sum_{j=0}^{N-1} \frac{\exp(B_j)}{1+\exp(B_j)} \nabla_p B_j = \frac{1}{\sigma^2}\sum_{j=0}^{N-1} \frac{\exp(B_j)}{1+\exp(B_j)} \sum_{d=0}^{D-1} W_{Dp+d,j}\hat{n}_d \\
&= \frac{1}{\sigma^2}\sum_{j=0}^{N-1}\sum_{d=0}^{D-1} \frac{W_{Dp+d,j}}{\exp(-B_j)+1}\hat{n}_d \\
\nabla_p^2 B &= \frac{1}{\sigma^2}\nabla_p \cdot \sum_{j=0}^{N-1}\sum_{d=0}^{D-1} \frac{W_{Dp+d,j}}{\exp(-B_j)+1}\hat{n}_d = \frac{1}{\sigma^2}\sum_{j=0}^{N-1}\sum_{d=0}^{D-1} W_{Dp+d,j}\frac{\exp(-B_j)}{(\exp(-B_j)+1)^2}\nabla_p B_j \cdot \hat{n}_d \\
&= \frac{1}{\sigma^4}\sum_{j=0}^{N-1}\sum_{d=0}^{D-1} W^2_{Dp+d,j}\frac{\exp(-B_j)}{(\exp(-B_j)+1)^2}
\end{aligned}
$$

Derivative of the distance between particles p and q, r_{pq}:

$$
\begin{aligned}
r_{pq} &= \left(\sum_{d=0}^{D-1}(r_{p,d}-r_{q,d})^2\right)^{1/2} \\
\nabla_k r_{pq} &= \frac{1}{2}\left(\sum_{d=0}^{D-1}(r_{p,d}-r_{q,d})^2\right)^{-1/2} \nabla_k \left\{\sum_{d=0}^{D-1}(r_{p,d}-r_{q,d})^2\right\} \\
&= \frac{1}{2r_{pq}}\sum_{d=0}^{D-1} 2(r_{p,d}-r_{q,d})(\delta_{k,p}-\delta_{k,q})\hat{n}_d = \frac{\delta_{k,p}-\delta_{k,q}}{r_{pq}}\sum_{d=0}^{D-1}(r_{p,d}-r_{q,d})\hat{n}_d
\end{aligned}
$$

For bosons:

$$
\begin{aligned}
J_B(\vec{R}) &= \sum_{p<q} \ln\left(1 - \frac{a}{r_{pq}}\right) \\
\nabla_k J_B &= \sum_{p<q} \frac{1}{1-\frac{a}{r_{pq}}} \nabla_k \left(1 - \frac{a}{r_{pq}}\right) = \sum_{p<q} \frac{r_{pq}}{r_{pq}-a}\frac{a}{r_{pq}^2}\nabla_k r_{pq} \\
&= \sum_{p<q} \frac{a}{r_{pq}(r_{pq}-a)}\frac{1}{r_{pq}} \sum_{d=0}^{D-1} (r_{p,d}-r_{q,d})(\delta_{k,p}-\delta_{k,q})\hat{n}_d \\
&= \frac{1}{2}\sum_{d=0}^{D-1}\sum_{p\neq q} \frac{a(r_{p,d}-r_{q,d})}{r_{pq}^2(r_{pq}-a)}(\delta_{k,p}-\delta_{k,q})\hat{n}_d \\
&= \frac{1}{2}\sum_{d=0}^{D-1}\left[\sum_{p\neq q} \frac{a(r_{p,d}-r_{q,d})}{r_{pq}^2(r_{pq}-a)}\delta_{k,p} - \sum_{p\neq q} \frac{a(r_{p,d}-r_{q,d})}{r_{pq}^2(r_{pq}-a)}\delta_{k,q}\right]\hat{n}_d \\
&= \frac{1}{2}\sum_{d=0}^{D-1}\left[\sum_{q\neq k} \frac{a(r_{k,d}-r_{q,d})}{r_{kq}^2(r_{kq}-a)} - \sum_{p\neq k} \frac{a(r_{p,d}-r_{k,d})}{r_{pk}^2(r_{pk}-a)}\right]\hat{n}_d \\
&= \frac{1}{2}\sum_{d=0}^{D-1}\left[2\sum_{p\neq k} \frac{a(r_{k,d}-r_{p,d})}{r_{kp}^2(r_{kp}-a)}\right]\hat{n}_d = a\sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1} \frac{r_{k,d}-r_{p,d}}{r_{kp}^2(r_{kp}-a)}\hat{n}_d \\
\nabla_k^2 J_B &= a\sum_{d=0}^{D-1}\hat{n}_d\frac{\partial}{\partial r_{k,d}} \cdot \sum_{d'=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1} \frac{r_{k,d'}-r_{p,d'}}{r_{kp}^2(r_{kp}-a)}\hat{n}_{d'} \\
&= a\sum_{d=0}^{D-1}\sum_{d'=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1} \frac{\partial}{\partial r_{k,d}}\left\{\frac{r_{k,d'}-r_{p,d'}}{r_{kp}^2(r_{kp}-a)}\right\}\delta_{d',d} \\
&= a\sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1} \frac{\partial}{\partial r_{k,d}}\left\{\frac{r_{k,d}-r_{p,d}}{r_{kp}^2(r_{kp}-a)}\right\} \\
&= a\sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1} \left[(r_{k,d}-r_{p,d})\frac{\partial}{\partial r_{k,d}}\left\{\frac{1}{r_{kp}^2(r_{kp}-a)}\right\} + \frac{\partial}{\partial r_{k,d}}\left\{r_{k,d}-r_{p,d}\right\}\frac{1}{r_{kp}^2(r_{kp}-a)}\right] \\
&= a\sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1} \left[(r_{k,d}-r_{p,d})\left[\frac{1}{r_{kp}^2}\frac{\partial}{\partial r_{k,d}}\left\{\frac{1}{r_{kp}-a}\right\} + \frac{\partial}{\partial r_{k,d}}\left\{\frac{1}{r_{kp}^2}\right\}\frac{1}{r_{kp}-a}\right] + \frac{1}{r_{kp}^2(r_{kp}-a)}\right] \\
&= a\sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1} \left[(r_{k,d}-r_{p,d})\frac{\partial r_{kp}}{\partial r_{k,d}}\left[\frac{-1}{r_{kp}^2(r_{kp}-a)^2} + \frac{-2}{r_{kp}^3}\frac{1}{r_{kp}-a}\right] + \frac{1}{r_{kp}^2(r_{kp}-a)}\right] \\
&= a\sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1} \frac{1}{r_{kp}^2(r_{kp}-a)}\left[\frac{(r_{k,d}-r_{p,d})^2}{r_{kp}}\left[\frac{-1}{r_{kp}-a} + \frac{-2}{r_{kp}}\right] + 1\right] \\
&= a\sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1} \frac{1}{r_{kp}^2(r_{kp}-a)}\left[\frac{(r_{k,d}-r_{p,d})^2}{r_{kp}}\left[\frac{2a-3r_{kp}}{r_{kp}(r_{kp}-a)}\right] + 1\right] \\
&= a\sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1} \frac{1}{r_{kp}^2(r_{kp}-a)}\left[\frac{(r_{k,d}-r_{p,d})^2(2a-3r_{kp})}{r_{kp}^2(r_{kp}-a)} + 1\right]
\end{aligned}
$$

For charged particles:

$$
\begin{aligned}
J_C(\vec{R}) &= \sum_{p<q} r_{pq} \\
\nabla_k J_C &= \sum_{p<q} \nabla_k r_{pq} = \sum_{p<q} \frac{\delta_{k,p} - \delta_{k,q}}{r_{pq}} \sum_{d=0}^{D-1} (r_{p,d} - r_{q,d}) \hat{n}_d \\
&= \frac{1}{2} \sum_{p \neq q} \frac{\delta_{k,p}}{r_{pq}} \sum_{d=0}^{D-1} (r_{p,d} - r_{q,d}) \hat{n}_d - \frac{1}{2} \sum_{p \neq q} \frac{\delta_{k,q}}{r_{pq}} \sum_{d=0}^{D-1} (r_{p,d} - r_{q,d}) \hat{n}_d \\
&= \frac{1}{2} \sum_{q \neq k} \frac{1}{r_{kq}} \sum_{d=0}^{D-1} (r_{k,d} - r_{q,d}) \hat{n}_d + \frac{1}{2} \sum_{p \neq k} \frac{1}{r_{pk}} \sum_{d=0}^{D-1} (r_{k,d} - r_{p,d}) \hat{n}_d = \sum_{d=0}^{D-1} \sum_{p \neq k} \frac{r_{k,d} - r_{p,d}}{r_{kp}} \hat{n}_d \\
\nabla_k^2 J_C &= \sum_{d=0}^{D-1} \sum_{p \neq k} \left[(r_{k,d} - r_{p,d}) \frac{\partial}{\partial r_{k,d}} \left\{ \frac{1}{r_{kp}} \right\} + \frac{\partial}{\partial r_{k,d}} \left\{ r_{k,d} - r_{p,d} \right\} \frac{1}{r_{kp}} \right] \\
&= \sum_{d=0}^{D-1} \sum_{p \neq k} \left[-\frac{(r_{k,d} - r_{p,d})}{r_{kp}^2} \frac{\partial r_{kp}}{\partial r_{k,d}} + \frac{1}{r_{kp}} \right] = \sum_{d=0}^{D-1} \sum_{p \neq k} \left[-\frac{(r_{k,d} - r_{p,d})}{r_{kp}^2} \frac{(r_{k,d} - r_{p,d})}{r_{kp}} + \frac{1}{r_{kp}} \right] \\
&= \sum_{d=0}^{D-1} \sum_{p \neq k} \frac{1}{r_{kp}} \left[1 - \frac{(r_{k,d} - r_{p,d})^2}{r_{kp}^2} \right] = \sum_{p \neq k} \frac{1}{r_{kp}} \left[D - \frac{1}{r_{kp}^2} \sum_{d=0}^{D-1} (r_{k,d} - r_{p,d})^2 \right] = (D-1) \sum_{p \neq k} \frac{1}{r_{kp}}
\end{aligned}
$$

Depending on what type of particles we have, substitute J with J_B or J_C. Putting all this together...

$$
\begin{aligned}
E_L &= \frac{1}{\Psi} \left[\frac{1}{2} \sum_{p=0}^{P-1} -\nabla_p^2 + \frac{1}{2} \sum_{d=0}^{D-1} \omega_d^2 r_{p,d}^2 \right] \Psi = -\frac{1}{2} \sum_{p=0}^{P-1} \frac{1}{\Psi} \nabla_p^2 \Psi + \frac{1}{2} \sum_{p=0}^{P-1} \sum_{d=0}^{D-1} \omega_d^2 r_{p,d}^2 \\
&= -\frac{1}{2} \sum_{p=0}^{P-1} \left[\nabla_p^2 A + \nabla_p^2 B + \nabla_p^2 J + \Big(\nabla_p A + \nabla_p B + \nabla_p J \Big)^2 \right] + \frac{1}{2} \sum_{p=0}^{P-1} \sum_{d=0}^{D-1} \omega_d^2 r_{p,d}^2 \\
&= -\frac{1}{2} \sum_{p=0}^{P-1} \Bigg[-\frac{D}{\sigma^2} + \frac{1}{\sigma^4} \sum_{j=0}^{N-1} \sum_{d=0}^{D-1} W_{Dp+d,j}^2 \frac{\exp(-B_j)}{(\exp(-B_j)+1)^2} + \nabla_p^2 J \\
&\qquad + \left(\frac{1}{\sigma^2} \sum_{d=0}^{D-1} (a_{Dp+d} - r_{p,d}) \hat{n_d} + \frac{1}{\sigma^2} \sum_{j=0}^{N-1} \sum_{d=0}^{D-1} \frac{W_{Dp+d,j}}{\exp(-B_j)+1} \hat{n}_d + \nabla_p J \right)^2 \Bigg] + \frac{1}{2} \sum_{p=0}^{P-1} \sum_{d=0}^{D-1} \omega_d^2 r_{p,d}^2 \\
&= \frac{PD}{2\sigma^2} - \frac{1}{2\sigma^4} \sum_{p=0}^{P-1} \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} W_{Dp+d,j}^2 \frac{\exp(-B_j)}{(\exp(-B_j)+1)^2} - \frac{1}{2} \sum_{p=0}^{P-1} \nabla_p^2 J \\
&\quad - \frac{1}{2} \sum_{p=0}^{P-1} \left(\frac{1}{\sigma^2} \sum_{d=0}^{D-1} (a_{Dp+d} - r_{p,d}) \hat{n_d} + \frac{1}{\sigma^2} \sum_{d=0}^{D-1} \sum_{j=0}^{N-1} \frac{W_{Dp+d,j}}{\exp(-B_j)+1} \hat{n}_d + \nabla_p J \right)^2 + \frac{1}{2} \sum_{p=0}^{P-1} \sum_{d=0}^{D-1} \omega_d^2 r_{p,d}^2
\end{aligned}
$$

Let's write the local energy in terms of our RBM inputs $\vec{x}$, i.e. switch from sums over particles and dimensions to sums over inputs. Here, I'll define some vectors that will make computation of the local energy simpler and faster. Store the quantities B_j in a vector called $\vec{B} \in \mathbb{R}^N$ (not to be confused with the function $B(\vec{R})$), and store the quantities

$$f_j = \frac{1}{\exp(-B_j) + 1}$$

in a vector $\vec{f} \in \mathbb{R}^N$. In the code, $\vec{f}$ is called sigmoid$B$. Also, store the squares of the frequencies and positions in vectors $\vec{\Omega^2}, \vec{x^2} \in \mathbb{R}^M$,

$$\begin{aligned}
(\Omega^2)_i &= (\omega_{i \bmod D})^2 \\
(x^2)_i &= x_i^2
\end{aligned}$$

so that the last double sum in the local energy becomes a simple dot product. Then the local energy becomes:

$$\begin{aligned}
E_L &= \frac{M}{2\sigma^2} - \frac{1}{2}\sum_{j=0}^{N-1} \exp(-B_j)\left\|\frac{f_j \vec{W}_j}{\sigma^2}\right\|^2 - \frac{1}{2}\sum_{p=0}^{P-1} \nabla_p^2 J \\
&\quad - \frac{1}{2}\sum_{p=0}^{P-1}\left(\frac{1}{\sigma^2}\sum_{d=0}^{D-1}\left(a_{Dp+d} - x_{Dp+d} + \vec{W}_{Dp+d}^T \vec{f}\right)\hat{n}_d + \nabla_p J\right)^2 + \frac{1}{2}\vec{\Omega^2} \cdot \vec{x^2} \\
&= \frac{1}{2}\Bigg[\frac{M}{\sigma^2} - \sum_{j=0}^{N-1} \exp(-B_j)\left\|\frac{f_j \vec{W}_j}{\sigma^2}\right\|^2 - \sum_{p=0}^{P-1} \nabla_p^2 J \\
&\quad - \sum_{p=0}^{P-1}\left(\frac{1}{\sigma^2}\sum_{d=0}^{D-1}\left(a_{Dp+d} - x_{Dp+d} + \vec{W}_{Dp+d}^T \vec{f}\right)\hat{n}_d + \nabla_p J\right)^2 + \vec{\Omega^2} \cdot \vec{x^2}\Bigg]
\end{aligned}$$

Putting all this together...

$$
\begin{aligned}
= -\frac{1}{2}\sum_{k=0}^{P-1}\Bigg(& -\frac{D}{\sigma^2} + \frac{1}{\sigma^4}\sum_{j=0}^{N-1}\frac{\exp(-B_j)}{(\exp(-B_j)+1)^2}\sum_{d=0}^{D-1}W_{Dk+d,j}^2 \\
& + \sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1}\frac{1}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\left[\left(\frac{r_{k,d}-r_{p,d}}{r_{kp}}\right)^2\frac{2a-3r_{kp}}{r_{kp}-a}+1\right] \\
& + \left(\frac{1}{\sigma^2}\sum_{d=0}^{D-1}(a_{Dk+d}-r_{k,d})\hat{n_d} + \frac{1}{\sigma^2}\sum_{d=0}^{D-1}\sum_{j=0}^{N-1}\frac{W_{Dk+d,j}}{\exp(-B_j)+1}\hat{n}_d + \sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1}\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\hat{n}_d\right)^2\Bigg) \\
+ \frac{1}{2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1}\omega_d^2 r_{p,d}^2 &
\end{aligned}
$$

$$
\begin{aligned}
= -\frac{1}{2}\sum_{k=0}^{P-1}\Bigg(& \sum_{d=0}^{D-1}\left[\frac{1}{\sigma^4}\sum_{j=0}^{N-1}\frac{\exp(-B_j)W_{Dk+d,j}^2}{(\exp(-B_j)+1)^2} + \sum_{p=0,\ p\neq k}^{P-1}\frac{1}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\left[\left(\frac{r_{k,d}-r_{p,d}}{r_{kp}}\right)^2\frac{2a-3r_{kp}}{r_{kp}-a}+1\right]\right] \\
& + \left(\sum_{d=0}^{D-1}\left[\frac{1}{\sigma^2}(a_{Dk+d}-r_{k,d}) + \frac{1}{\sigma^2}\sum_{j=0}^{N-1}\frac{W_{Dk+d,j}}{\exp(-B_j)+1} + \sum_{p=0,\ p\neq k}^{P-1}\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\right]\hat{n}_d\right)^2\Bigg) \\
+ \frac{PD}{2\sigma^2} + \frac{1}{2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1}\omega_d^2 r_{p,d}^2 &
\end{aligned}
$$

$$
\begin{aligned}
= -\frac{1}{2}\sum_{k=0}^{P-1}\sum_{d=0}^{D-1}\Bigg[& \frac{1}{\sigma^4}\sum_{j=0}^{N-1}\frac{\exp(-B_j)W_{Dk+d,j}^2}{(\exp(-B_j)+1)^2} + \sum_{p=0,\ p\neq k}^{P-1}\frac{1}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\left[\left(\frac{r_{k,d}-r_{p,d}}{r_{kp}}\right)^2\frac{2a-3r_{kp}}{r_{kp}-a}+1\right] \\
& + \left(\frac{1}{\sigma^2}(a_{Dk+d}-r_{k,d}) + \frac{1}{\sigma^2}\sum_{j=0}^{N-1}\frac{W_{Dk+d,j}}{\exp(-B_j)+1} + \sum_{p=0,\ p\neq k}^{P-1}\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\right)^2\Bigg] \\
+ \frac{PD}{2\sigma^2} + \frac{1}{2}\sum_{p=0}^{P-1}\sum_{d=0}^{D-1}\omega_d^2 r_{p,d}^2 &
\end{aligned}
$$

To write E_L in terms of the inputs x_i, we define the distance between the kth and pth particle as

$$
\begin{aligned}
R_i(p) \equiv r_{kp} &= \left(\sum_{d=0}^{D-1}(r_{k,d}-r_{p,d})^2\right)^{1/2} \\
&= r_{(\text{floor}(i/D))p} = \left(\sum_{d=0}^{D-1}(x_{D(\text{floor}(i/D))+d}-x_{Dp+d})^2\right)^{1/2}
\end{aligned}
$$

Then,

$$
\begin{aligned}
E_L = &-\frac{1}{2}\sum_{i=0}^{M-1}\Bigg[\frac{1}{\sigma^4}\sum_{j=0}^{N-1}\frac{\exp(-B_j)W_{i,j}^2}{(\exp(-B_j)+1)^2} \\
&\qquad + a\sum_{p=0,\ p\neq \mathrm{floor}(i/D)}^{P-1}\frac{1}{R_i(p)^2\big(R_i(p)-a\big)}\bigg[\Big(\frac{x_i - x_{Dp+(i \mathrm{mod} D)}}{R_i(p)}\Big)^2\frac{2a-3R_i(p)}{R_i(p)-a}+1\bigg] \\
&\qquad + \left(\frac{1}{\sigma^2}(a_i - x_i) + \frac{1}{\sigma^2}\sum_{j=0}^{N-1}\frac{W_{i,j}}{\exp(-B_j)+1} + a\sum_{p=0,\ p\neq \mathrm{floor}(i/D)}^{P-1}\frac{x_i - x_{Dp+(i \mathrm{mod} D)}}{R_i(p)^2\left(R_i(p)-a\right)}\right)^2\Bigg] \\
&+\frac{M}{2\sigma^2}+\frac{1}{2}\sum_{i=0}^{M-1}\omega_{i \mathrm{mod} D}^2 x_i^2
\end{aligned}
$$

$$
\begin{aligned}
= &-\frac{1}{2\sigma^4}\sum_{j=0}^{N-1}\frac{\exp(-B_j)}{(\exp(-B_j)+1)^2}\sum_{i=0}^{M-1}W_{i,j}^2 \\
&-\frac{a}{2}\sum_{i=0}^{M-1}\sum_{p=0,\ p\neq \mathrm{floor}(i/D)}^{P-1}\frac{1}{R_i(p)^2\big(R_i(p)-a\big)}\bigg[\Big(\frac{x_i - x_{Dp+(i \mathrm{mod} D)}}{R_i(p)}\Big)^2\frac{2a-3R_i(p)}{R_i(p)-a}+1\bigg] \\
&-\frac{1}{2}\sum_{i=0}^{M-1}\left(\frac{1}{\sigma^2}(a_i - x_i) + \frac{1}{\sigma^2}\sum_{j=0}^{N-1}\frac{W_{i,j}}{\exp(-B_j)+1} + a\sum_{p=0,\ p\neq \mathrm{floor}(i/D)}^{P-1}\frac{x_i - x_{Dp+(i \mathrm{mod} D)}}{R_i(p)^2\left(R_i(p)-a\right)}\right)^2 \\
&+\frac{M}{2\sigma^2}+\frac{1}{2}\sum_{i=0}^{M-1}\omega_{i \mathrm{mod} D}^2 x_i^2
\end{aligned}
$$

$$
\begin{aligned}
= &-\frac{1}{2\sigma^4}\sum_{j=0}^{N-1}\frac{\exp(-B_j)}{(\exp(-B_j)+1)^2}\vec{W}_j\cdot\vec{W}_j \\
&-\frac{a}{2}\sum_{i=0}^{M-1}\sum_{p=0,\ p\neq \mathrm{floor}(i/D)}^{P-1}\frac{1}{R_i(p)^2\big(R_i(p)-a\big)}\bigg[\Big(\frac{x_i - x_{Dp+(i \mathrm{mod} D)}}{R_i(p)}\Big)^2\frac{2a-3R_i(p)}{R_i(p)-a}+1\bigg] \\
&-\frac{1}{2}\sum_{i=0}^{M-1}\left(\frac{1}{\sigma^2}(a_i - x_i) + \frac{1}{\sigma^2}\sum_{j=0}^{N-1}\frac{W_{i,j}}{\exp(-B_j)+1} + a\sum_{p=0,\ p\neq \mathrm{floor}(i/D)}^{P-1}\frac{x_i - x_{Dp+(i \mathrm{mod} D)}}{R_i(p)^2\left(R_i(p)-a\right)}\right)^2 \\
&+\frac{M}{2\sigma^2}+\frac{1}{2}(\Omega\%\Omega)\cdot(\vec{x}\%\vec{x})
\end{aligned}
$$

In the last line, we have defined a vector $\vec{\Omega}$ with elements $\Omega_i = \omega_{i \mathrm{mod} D}$. To increase the computational speed, we will precalculate and store the values B_j in a vector $\vec{B}$ and store the following factors in a vector $\vec{f} \in \mathbb{R}^N$:

$$f_j \equiv \frac{1}{\exp(-B_j)+1}$$

Then, the local energy becomes

$$
\begin{aligned}
E_L = & -\frac{1}{2}\sum_{j=0}^{N-1}\exp(-B_j)\left\|\frac{f_j\vec{W}_j}{\sigma^2}\right\|^2 + \frac{M}{2\sigma^2} + \frac{1}{2}(\Omega\%\Omega)\cdot(\vec{x}\%\vec{x}) \\
& -\frac{a}{2}\sum_{i=0}^{M-1}\sum_{p=0,\ p\neq \text{floor}(i/D)}^{P-1}\frac{1}{R_i(p)^2\big(R_i(p)-a\big)}\Big[\Big(\frac{x_i - x_{Dp+(i\text{mod}D)}}{R_i(p)}\Big)^2\frac{2a-3R_i(p)}{R_i(p)-a}+1\Big] \\
& -\frac{1}{2}\sum_{i=0}^{M-1}\left(\frac{1}{\sigma^2}(a_i - x_i) + \frac{1}{\sigma^2}\vec{W}_i^T\vec{f} + a\sum_{p=0,\ p\neq \text{floor}(i/D)}^{P-1}\frac{x_i - x_{Dp+(i\text{mod}D)}}{R_i(p)^2\left(R_i(p)-a\right)}\right)^2
\end{aligned}
$$

For stochastic gradient descent, we will also need the gradient of the local energy with respect to the RBM parameters $\vec{\theta} = (\vec{a}, \vec{b}, \hat{W})$:

$$
G_k = \frac{\partial\langle E_L\rangle}{\partial\theta_k} = 2\left(\left\langle E_L\frac{1}{\Psi}\frac{\partial\Psi}{\partial\theta_k}\right\rangle - \langle E_L\rangle\left\langle\frac{1}{\Psi}\frac{\partial\Psi}{\partial\theta_k}\right\rangle\right)
$$

The derivatives of our new wavefunction with respect to the variational parameters are given by:

$$
\begin{aligned}
\frac{\partial\Psi}{\partial\vec{a}} &= \Psi\frac{\partial A(\vec{a})}{\partial\vec{a}} = \Psi\frac{\vec{x}-\vec{a}}{\sigma^2} \\
\frac{\partial\Psi}{\partial\vec{b}} &= \Psi\frac{\partial B(\vec{b},\hat{W})}{\partial\vec{b}} = \Psi\vec{f} \\
\frac{\partial\Psi}{\partial\hat{W}} &= \Psi\frac{\partial B(\vec{b},\hat{W})}{\partial\hat{W}} = \Psi\frac{\vec{x}\vec{f}^T}{\sigma^2}
\end{aligned}
$$

The quantum force on the kth particle is defined as

$$
\vec{F}_k(\vec{R}) = 2\frac{1}{\Psi}\nabla_k\Psi. \tag{1}
$$

Using the derivatives we have already calculated, we have

$$
\begin{aligned}
\vec{F}_k(\vec{R}) &= 2\Big(\nabla_k\{A\} + \nabla_k\{B\} + \nabla_k\{J\}\Big) \\
&= 2\left(\frac{1}{\sigma^2}\sum_{d=0}^{D-1}(a_{Dk+d} - r_{k,d})\hat{n}_d + \frac{1}{\sigma^2}\sum_{d=0}^{D-1}\sum_{j=0}^{N-1}\frac{W_{Dk+d,j}}{\exp(-B_j)+1}\hat{n}_d + \sum_{d=0}^{D-1}\sum_{p=0,\ p\neq k}^{P-1}\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\hat{n}_d\right) \\
&= 2\sum_{d=0}^{D-1}\left[\frac{1}{\sigma^2}(a_{Dk+d} - r_{k,d}) + \frac{1}{\sigma^2}\vec{W}_{Dk+d}^T\vec{f} + \sum_{p=0,\ p\neq k}^{P-1}\frac{r_{k,d}-r_{p,d}}{r_{kp}^2\left(\frac{r_{kp}}{a}-1\right)}\right]\hat{n}_d
\end{aligned}
$$

The Langevin and Fokker-Planck equations give a new position y from the old position x:

$$
y = x + d\Delta t F(x) + \xi\sqrt{\Delta t}, \tag{2}
$$

where $d = 0.5$ is the diffusion constant and $\Delta t \in [0.001, 0.01]$ is a chosen time step.

The transition probability is given by the Green's function

$$G(y,x) = \frac{1}{(4\pi d\Delta t)^{3N/2}} \exp\left(-\frac{(y-x-d\Delta t F(x))^2}{4d\Delta t}\right), \tag{3}$$

so that the Metropolis-Hastings acceptance ratio is

$$A(y,x) = \min\{1, P(y,x)\}, \tag{4}$$

where

$$\begin{aligned}
P(y,x) &= \frac{G(x,y)|\Psi_T(y)|^2}{G(y,x)|\Psi_T(x)|^2} \\
&= \exp\left(-\frac{(x-y-d\Delta t F(y))^2}{4d\Delta t}\right) \exp\left(\frac{(y-x-d\Delta t F(x))^2}{4d\Delta t}\right) \frac{|\Psi_T(y)|^2}{|\Psi_T(x)|^2} \\
&= \exp\left(-\frac{(x-y)^2 - 2(x-y)d\Delta t F(y) + d^2\Delta t^2 F(y)^2}{4d\Delta t}\right) \\
&\quad \times \exp\left(\frac{(y-x)^2 - 2(y-x)d\Delta t F(x) + d^2\Delta t^2 F(x)^2}{4d\Delta t}\right) \frac{|\Psi_T(y)|^2}{|\Psi_T(x)|^2} \\
&= \exp\left(\frac{2(x-y)d\Delta t(F(y)+F(x)) + d^2\Delta t^2(F(x)^2 - F(y)^2)}{4d\Delta t}\right) \frac{|\Psi_T(y)|^2}{|\Psi_T(x)|^2} \\
&= \exp\left(\frac{2(x-y)(F(y)+F(x)) + d\Delta t(F(x)^2 - F(y)^2)}{4}\right) \frac{|\Psi_T(y)|^2}{|\Psi_T(x)|^2} \\
&= \exp\left(\frac{1}{2}(x-y)(F(y)+F(x)) + \frac{1}{4}d\Delta t(F(x)^2 - F(y)^2)\right) \frac{|\Psi_T(y)|^2}{|\Psi_T(x)|^2}
\end{aligned}$$