BOSONS

Hamiltonian of N D-dimensional bosons in harmonic oscillator potential with hard-sphere interaction ($\hbar = m = 1$):

$$\hat{H} = \sum_{i=1}^{N} \Big\{ -\frac{1}{2}\nabla_i^2 + \frac{1}{2}(\omega_1^2 r_{i,1}^2 + \cdots + \omega_D^2 r_{i,D}^2) \Big\} + \sum_{i<j}^{N} V_{int}(\vec{r_i}, \vec{r_j}), \tag{1}$$

$$V_{int}(\vec{r_i}, \vec{r_j}) = \begin{cases} \infty, & r_{ij} \leq a \\ 0, & r_{ij} > a \end{cases} \tag{2}$$

Store the squares of the harmonic oscillator frequencies in a vector of size D so we can write $\hat{H}$ as:

$$\hat{H} = \frac{1}{2}\sum_{i=1}^{N} \Big\{ -\nabla_i^2 + \vec{\omega^2} \cdot \vec{r_i^2} \Big\}, \tag{3}$$

$$\vec{\omega^2} = \vec{\omega} \ \% \ \vec{\omega} = \langle \omega_1^2, \cdots, \omega_D^2 \rangle \tag{4}$$

$$\vec{r_i^2} = \vec{r_i} \ \% \ \vec{r_i} = \langle r_{i,1}^2, \cdots, r_{i,D}^2 \rangle \tag{5}$$

$$\tag{6}$$

The interaction is taken care of by forcing the trial wavefunction to vanish if any two bosons become separated by a distance less than a. Trial wavefunction:

$$\Psi_T(\vec{R}) = \Big\{ \prod_{i=1}^{N} \exp(-\vec{\alpha} \cdot \vec{r_i^2}) \Big\} \Big\{ \prod_{i<j}^{N} \exp\left(\ln\left(1 - \frac{a}{r_{ij}}\right)\right) \Big\} = \exp\Big(p(\vec{\alpha}, \vec{R}) + q(\vec{R}) \Big) \tag{7}$$

$$p(\vec{\alpha}, \vec{R}) = -\sum_{i=1}^{N} \vec{\alpha} \cdot \vec{r_i^2} \tag{8}$$

$$q(\vec{R}) = \sum_{i<j}^{N} \ln\left(1 - \frac{a}{r_{ij}}\right) \tag{9}$$

The local energy is defined as

$$E_L(\vec{R}) = \frac{1}{\Psi_T} \hat{H} \Psi_T \tag{10}$$

We need the following derivatives to obtain the analytical form of the local energy:

$$\frac{1}{\Psi_T}\nabla_i^2\Psi_T = \nabla_i^2 p + \nabla_i^2 q + (\nabla_i p + \nabla_i q)^2$$

$$\nabla_i p = -2\vec{\alpha} \,\%\, \vec{r_i}$$

$$\nabla_i^2 p = -2\vec{\alpha}\cdot\vec{\mathbb{1}}$$

$$\nabla_i q = \sum_{j\neq i}^{N} \frac{a}{r_{ij}^2(r_{ij}-a)}(\vec{r_i}-\vec{r_j})$$

$$\begin{aligned}
\nabla_i^2 q &= \nabla_i \cdot \left(\sum_{j\neq i}^{N} \frac{a}{r_{ij}^2(r_{ij}-a)}(\vec{r_i}-\vec{r_j})\right)\\
&= \sum_{d=1}^{D} \frac{\mathrm{d}}{\mathrm{d}r_{i,d}} \left(\sum_{j\neq i}^{N} \frac{a}{r_{ij}^2(r_{ij}-a)}(r_{i,d}-r_{j,d})\right)\\
&= \sum_{j\neq i}^{N}\sum_{d=1}^{D} \frac{\mathrm{d}}{\mathrm{d}r_{i,d}} \left(\frac{a}{r_{ij}^2(r_{ij}-a)}(r_{i,d}-r_{j,d})\right)\\
&= \sum_{j\neq i}^{N}\sum_{d=1}^{D} \left(-\frac{a(r_{i,d}-r_{j,d})^2}{r_{ij}^4(r_{ij}-a)^2}(3r_{ij}-2a) + \frac{a}{r_{ij}^2(r_{ij}-a)}\right)\\
&= \sum_{j\neq i}^{N} \left(\frac{aD}{r_{ij}^2(r_{ij}-a)} - \sum_{d=1}^{D} \frac{a(r_{i,d}-r_{j,d})^2}{r_{ij}^4(r_{ij}-a)^2}(3r_{ij}-2a)\right)\\
&= \sum_{j\neq i}^{N} \left(\frac{aD}{r_{ij}^2(r_{ij}-a)} - \frac{a(3r_{ij}-2a)}{r_{ij}^4(r_{ij}-a)^2}\left(\sum_{d=1}^{D}(r_{i,d}-r_{j,d})^2\right)\right)\\
&= \sum_{j\neq i}^{N} \left(\frac{aD}{r_{ij}^2(r_{ij}-a)} - \frac{a(3r_{ij}-2a)}{r_{ij}^2(r_{ij}-a)^2}\right)\\
&= \sum_{j\neq i}^{N} \frac{a}{r_{ij}^2(r_{ij}-a)}\left(D - \frac{3r_{ij}-2a}{r_{ij}-a}\right)\\
&= \sum_{j\neq i}^{N} \frac{a}{r_{ij}^2(r_{ij}-a)}\left(\frac{Dr_{ij}-Da-3r_{ij}+2a}{r_{ij}-a}\right)\\
&= \sum_{j\neq i}^{N} \frac{a}{r_{ij}^2(r_{ij}-a)}\left(\frac{(D-3)r_{ij}+(2-D)a}{r_{ij}-a}\right)\\
&= \sum_{j\neq i}^{N} \frac{a}{r_{ij}^2(r_{ij}-a)^2}\left((D-3)r_{ij}+(2-D)a\right)
\end{aligned}$$

$$\begin{aligned}
(\nabla_i p + \nabla_i q)^2 &= \left(-2\vec{\alpha}\,\%\,\vec{r_i} + \sum_{j\neq i}^{N} \frac{a(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)}\right)^2\\
&= 4\vec{\alpha^2}\cdot\vec{r_i^2} - 4a\sum_{j\neq i}^{N}\frac{(\vec{\alpha}\,\%\,\vec{r_i})\cdot(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)} + \left(\sum_{j\neq i}^{N}\frac{a(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)}\right)\cdot\left(\sum_{j\neq i}^{N}\frac{a(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)}\right)
\end{aligned}$$

Putting all this together...

$$
\begin{aligned}
E_L(\vec{R}) &= \frac{1}{\Psi_T}\left[\sum_{i=1}^{N}\Big\{-\frac{1}{2}\nabla_i^2 + \frac{1}{2}(\omega_1^2 r_{i,1}^2 + \cdots + \omega_D^2 r_{i,D}^2)\Big\}\right]\Psi_T \\
&= \frac{1}{2}\sum_{i=1}^{N}\Big\{-\frac{1}{\Psi_T}\nabla_i^2\Psi_T + \vec{\omega^2}\cdot\vec{r_i^2}\Big\} \\
&= \frac{1}{2}\sum_{i=1}^{N}\Big\{-\nabla_i^2 p - \nabla_i^2 q - (\nabla_i p + \nabla_i q)^2 + \vec{\omega^2}\cdot\vec{r_i^2}\Big\} \\
&= \frac{1}{2}\sum_{i=1}^{N}\Big\{2\vec{\alpha}\cdot\vec{\mathbb{1}} - \sum_{j\neq i}^{N}\frac{a}{r_{ij}^2(r_{ij}-a)^2}\left((D-3)r_{ij} + (2-D)a\right) - \\
&\quad \left[4\vec{\alpha^2}\cdot\vec{r_i^2} - 4a\sum_{j\neq i}^{N}\frac{(\vec{\alpha}\ \%\ \vec{r_i})\cdot(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)} + \left(\sum_{j\neq i}^{N}\frac{a(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)}\right)\cdot\left(\sum_{j\neq i}^{N}\frac{a(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)}\right)\right] + \vec{\omega^2}\cdot\vec{r_i^2}\Big\} \\
&= N\vec{\alpha}\cdot\vec{\mathbb{1}} - \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}\frac{a((D-3)r_{ij}+(2-D)a)}{r_{ij}^2(r_{ij}-a)^2} - 2\sum_{i=1}^{N}\vec{\alpha^2}\cdot\vec{r_i^2} + 2a\sum_{i=1}^{N}\sum_{j\neq i}^{N}\frac{(\vec{\alpha}\ \%\ \vec{r_i})(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)} \\
&\quad - \frac{1}{2}\sum_{i=1}^{N}\left(\sum_{j\neq i}^{N}\frac{a(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)}\right)\cdot\left(\sum_{j\neq i}^{N}\frac{a(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)}\right) + \frac{1}{2}\sum_{i=1}^{N}\vec{\omega^2}\cdot\vec{r_i^2} \\
&= N\vec{\alpha}\cdot\vec{\mathbb{1}} - 2\sum_{i=1}^{N}\vec{\alpha^2}\cdot\vec{r_i^2} + \sum_{i<j}^{N}\left[\frac{a((3-D)r_{ij}+(D-2)a)}{r_{ij}^2(r_{ij}-a)^2} + \frac{4a(\vec{\alpha}\ \%\ \vec{r_i})(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)}\right] \\
&\quad - \frac{1}{2}\sum_{i=1}^{N}\left(\sum_{j\neq i}^{N}\frac{a(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)}\right)\cdot\left(\sum_{j\neq i}^{N}\frac{a(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)}\right) + \frac{1}{2}\sum_{i=1}^{N}\vec{\omega^2}\cdot\vec{r_i^2} \\
&= N\vec{\alpha}\cdot\vec{\mathbb{1}} - 2\sum_{i=1}^{N}\vec{\alpha^2}\cdot\vec{r_i^2} + \sum_{i<j}^{N}\frac{a}{r_{ij}^2(r_{ij}-a)}\left[\frac{(3-D)r_{ij}+(D-2)a}{r_{ij}-a} + 4(\vec{\alpha}\ \%\ \vec{r_i})\cdot(\vec{r_i}-\vec{r_j})\right] \\
&\quad - \frac{1}{2}\sum_{i=1}^{N}\left(\sum_{j\neq i}^{N}\frac{a(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)}\right)\cdot\left(\sum_{j\neq i}^{N}\frac{a(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)}\right) + \frac{1}{2}\sum_{i=1}^{N}\vec{\omega^2}\cdot\vec{r_i^2}
\end{aligned}
$$

For importance sampling, we need the gradient of Ψ_T with respect to the variational parameters α_d, $d = 1, ..., D$.

$$\frac{\partial}{\partial\alpha_d}\Psi_T = \exp(p+q)\frac{\partial}{\partial\alpha_d}p = -\Psi_T\sum_{i=1}^{N} r_{i,d}^2$$

For gradient descent, we need an expression for the derivative of E_L with respect to the variational parameters $\vec{\alpha}$. We will only consider contributions from b particles in batch B_k, where k is chosen randomly. The variational parameters are only present in a few terms in the above expression for E_L, so we shall ignore the rest.

$$
\begin{aligned}
\frac{\partial E_L}{\partial \alpha_d} &= \frac{\partial}{\partial \alpha_d}\left(b\vec{\alpha}\cdot\vec{\mathbb{1}} - 2\sum_{i\in B_k}\vec{\alpha^2}\cdot\vec{r_i^2} + \sum_{i\in B_k}\frac{1}{2}\sum_{j\neq i}^{N}\frac{4a}{r_{ij}^2(r_{ij}-a)}(\vec{\alpha}\ \%\ \vec{r_i})\cdot(\vec{r_i}-\vec{r_j})\right)\\
&= b - 4\sum_{i\in B_k}\alpha_d r_{i,d}^2 + 2\sum_{i\in B_k}\sum_{j\neq i}^{N}\frac{a r_{i,d}(r_{i,d}-r_{j,d})}{r_{ij}^2(r_{ij}-a)}
\end{aligned}
$$

The quantum force on the ith particle is defined as

$$\vec{F_i}(\vec{R}) = 2\frac{1}{\Psi_T}\nabla_i\Psi_T. \tag{11}$$

Using the derivatives we have already calculated, we have

$$
\begin{aligned}
\vec{F_i}(\vec{R}) &= 2(\nabla_i p + \nabla_i q)\\
&= -4\vec{\alpha}\ \%\ \vec{r_i} + 2\sum_{j\neq i}^{N}\frac{a(\vec{r_i}-\vec{r_j})}{r_{ij}^2(r_{ij}-a)}
\end{aligned}
$$

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

$$y = x + d\Delta t F(x) + \xi\sqrt{\Delta t}, \tag{12}$$

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

$$G(y,x) = \frac{1}{(4\pi d\Delta t)^{3N/2}}\exp\left(-\frac{(y-x-d\Delta t F(x))^2}{4d\Delta t}\right), \tag{13}$$

so that the Metropolis-Hastings acceptance ratio is

$$A(y,x) = \min\{1, P(y,x)\}, \tag{14}$$

where

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