

BOSONS

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

$$\hat{H} = \sum_{i=1}^N \left\{ -\frac{1}{2} \nabla_i^2 + \frac{1}{2} (\omega_1^2 r_{i,1}^2 + \cdots + \omega_D^2 r_{i,D}^2) \right\} + \sum_{i < j}^N V_{int}(\vec{r}_i, \vec{r}_j), \quad (1)$$

$$V_{int}(\vec{r}_i, \vec{r}_j) = \begin{cases} \infty, & r_{ij} \leq a \\ 0, & r_{ij} > a \end{cases} \quad (2)$$

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

$$\hat{H} = \frac{1}{2} \sum_{i=1}^N \left\{ -\nabla_i^2 + \vec{\omega}^2 \cdot \vec{r}_i^2 \right\}, \quad (3)$$

$$\vec{\omega}^2 = \vec{\omega} \ \% \ \vec{\omega} = \langle \omega_1^2, \dots, \omega_D^2 \rangle \quad (4)$$

$$\vec{r}_i^2 = \vec{r}_i \ \% \ \vec{r}_i = \langle r_{i,1}^2, \dots, r_{i,D}^2 \rangle \quad (5)$$

$$(6)$$

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:

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

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

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

The local energy is defined as

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

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

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

$$\nabla_i p = -2\vec{\alpha} \% \vec{r}_i$$

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

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

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

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

Putting all this together...

$$\begin{aligned}
E_L(\vec{R}) &= \frac{1}{\Psi_T} \left[\sum_{i=1}^N \left\{ -\frac{1}{2} \nabla_i^2 + \frac{1}{2} (\omega_1^2 r_{i,1}^2 + \dots + \omega_D^2 r_{i,D}^2) \right\} \right] \Psi_T \\
&= \frac{1}{2} \sum_{i=1}^N \left\{ -\frac{1}{\Psi_T} \nabla_i^2 \Psi_T + \vec{\omega}^2 \cdot \vec{r}_i^2 \right\} \\
&= \frac{1}{2} \sum_{i=1}^N \left\{ -\nabla_i^2 p - \nabla_i^2 q - (\nabla_i p + \nabla_i q)^2 + \vec{\omega}^2 \cdot \vec{r}_i^2 \right\} \\
&= \frac{1}{2} \sum_{i=1}^N \left\{ 2\vec{\alpha} \cdot \vec{\mathbb{I}} - \sum_{j \neq i}^N \frac{a}{r_{ij}^2 (r_{ij} - a)^2} ((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 \right\} \\
&= N\vec{\alpha} \cdot \vec{\mathbb{I}} - \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) \cdot (\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{I}} - 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) \cdot (\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{I}} - 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 , $d = 1, \dots, D$.

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

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.

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

The quantum force on the i th particle is defined as

$$\vec{F}_i(\vec{R}) = 2 \frac{1}{\Psi_T} \nabla_i \Psi_T. \quad (11)$$

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 :

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

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

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

so that the Metropolis-Hastings acceptance ratio is

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

where

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