

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:

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