To calculate matrix elements we use a linear sum of Gaussian basis function of the form

$$\psi = \psi^x \psi^y \psi^z$$

$$\psi^x(\boldsymbol{x}, A^x) = exp\left(-\frac{1}{2}\boldsymbol{x}^T A^x \boldsymbol{x}\right)$$

Where $\boldsymbol{x}^T = (x_1, x_2, \dots . x_N)$. And A^x is symmetric positive defined $N \times N$ matrix.

denote $\mathbb{A}_x = A'_x + A_x$ we get

(1) $\langle \psi'^x | \psi^x \rangle = \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}_x}}$

(2) $\langle \psi'^x | x_1 x_2 | \psi^x \rangle = \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}_x}} (\mathbb{A}_x^{-1})_{21}$

(3) $\langle \psi'^x | x_1^2 | \psi^x \rangle = \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}_x}} (\mathbb{A}_x^{-1})_{11}$

(4) $\left\langle \psi'^x \middle| \frac{\partial}{\partial x_1}\frac{\partial}{\partial x_2} \middle| \psi^x \right\rangle = \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}_x}} \left(-A_{21}^x + \sum_{ij} A_{2i}^x A_{1j}^x \,(\mathbb{A}_x^{-1})_{ij}\right)$

(5) $\left\langle \psi'^x \middle| \frac{\partial^2}{\partial x_1^2} \middle| \psi^x \right\rangle = -\sqrt{\frac{(2\pi)^N}{\det \mathbb{A}_x}} \sum_{ij} A'^x_{1i} A_{1j}^x \,(\mathbb{A}_x^{-1})_{ij} = \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}_x}} \left(-A_{11}^x + \sum_{ij} A_{1i}^x A_{1j}^x \,(\mathbb{A}_x^{-1})_{ij}\right)$

(6) $\left\langle \psi'^x \middle| x_1 \frac{\partial}{\partial x_2} \middle| \psi^x \right\rangle = -\sqrt{\frac{(2\pi)^N}{\det \mathbb{A}_x}} \sum_i A_{2i}^x \,(\mathbb{A}_x^{-1})_{1i}$

(7) $\left\langle \psi'^x \middle| x_1 \frac{\partial}{\partial x_1} \middle| \psi^x \right\rangle = -\sqrt{\frac{(2\pi)^N}{\det \mathbb{A}_x}} \sum_i A_{1i}^x \,(\mathbb{A}_x^{-1})_{1i}$

(8) $\left\langle \psi'^x \middle| \frac{\partial}{\partial x_1} x_1 \middle| \psi^x \right\rangle = \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}_x}} (1 - (\mathbb{A}_x^{-1})_{11} \sum_i A_{1i}^x)$

CALCULATION

=======calculation for 1,2,3================

Denote $\int d\boldsymbol{x} = \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dx_1 \dots dx_N$

$$\int d\boldsymbol{x}\ exp\left(-\frac{1}{2}\boldsymbol{x}^T A \boldsymbol{x} + \boldsymbol{b}\cdot\boldsymbol{x}\right) = \sqrt{\frac{(2\pi)^N}{\det A}}\, exp\left(\frac{1}{2}\boldsymbol{b}^T A^{-1}\boldsymbol{b}\right)$$

$$\int d\boldsymbol{x}\ x_1 x_2 exp\left(-\frac{1}{2}\boldsymbol{x}^T A \boldsymbol{x} + \boldsymbol{b}\cdot\boldsymbol{x}\right) = \frac{\partial}{\partial b_1}\frac{\partial}{\partial b_2}\int d\boldsymbol{x}\, exp\left(-\frac{1}{2}\boldsymbol{x}^T A \boldsymbol{x} + \boldsymbol{b}\cdot\boldsymbol{x}\right)$$

$$= \frac{\partial}{\partial b_1}\frac{\partial}{\partial b_2}\sqrt{\frac{(2\pi)^N}{\det A}}\, exp\left(\frac{1}{2}\boldsymbol{b}^T A^{-1}\boldsymbol{b}\right) = \frac{\partial}{\partial b_1}\sqrt{\frac{(2\pi)^N}{\det A}}\, exp\left(\frac{1}{2}\boldsymbol{b}^T A^{-1}\boldsymbol{b}\right)(A^{-1}\boldsymbol{b})_2$$

$$= \sqrt{\frac{(2\pi)^N}{\det A}} exp\left(\frac{1}{2}\boldsymbol{b}^T A^{-1}\boldsymbol{b}\right)\left[(A^{-1}\boldsymbol{b})_i^2 + (A^{-1})_{21}\right]$$

======calculation for 4,5===========

$$\int d\boldsymbol{x}\ \frac{\partial}{\partial x_1}\frac{\partial}{\partial x_2} exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right) = -\int d\boldsymbol{x}\ \frac{\partial}{\partial x_1}(A\boldsymbol{x})_2 exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right)$$

$$= -\int d\boldsymbol{x}\,(\,A_{21} - (A\boldsymbol{x})_2(A\boldsymbol{x})_1) exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right) = \sqrt{\frac{(2\pi)^N}{\det A}}\left(-A_{21} + \sum_{ij} A_{2i}A_{1j}\,(A^{-1})_{ij}\right)$$

========calculation of 4 by integration by part=========

$$\int d\boldsymbol{x} exp\left(-\frac{1}{2}\boldsymbol{x}^T A'\boldsymbol{x}\right)\frac{\partial^2}{\partial x_1^2} exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right)$$

$$= -\int d\boldsymbol{x}\ \left(\frac{\partial}{\partial x_1} exp\left(-\frac{1}{2}\boldsymbol{x}^T A'\boldsymbol{x}\right)\right)\left(\frac{\partial}{\partial x_1} exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right)\right)$$

$$= -\int d\boldsymbol{x}\left((A'\boldsymbol{x})_1 exp\left(-\frac{1}{2}\boldsymbol{x}^T A'\boldsymbol{x}\right)\right)\left((A\boldsymbol{x})_1 exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right)\right)$$

$$= -\int d\boldsymbol{x}\ \ (A'\boldsymbol{x})_1(A\boldsymbol{x})_1 exp\left(-\frac{1}{2}\boldsymbol{x}^T \mathbb{A}\boldsymbol{x}\right) = -\sum_{ij} A'_{1i}A_{1j}\int d\boldsymbol{x}\ \ x_i x_j exp\left(-\frac{1}{2}\boldsymbol{x}^T \mathbb{A}\boldsymbol{x}\right)$$

$$= -\sqrt{\frac{(2\pi)^N}{det\mathbb{A}}}\left(\sum_{ij} A'_{1i}A_{1j}\,(\mathbb{A}^{-1})_{ij}\right)$$

==========calculation for 6,7===========

$$\int d\boldsymbol{x}\ \ x_1\frac{\partial}{\partial x_2} exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right) = -\int d\boldsymbol{x}\ \ x_1(A\boldsymbol{x})_2 exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right)$$

$$= -\sum_i A_{2i}\int d\boldsymbol{x}\ \ x_1 x_i exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right) = -\sqrt{\frac{(2\pi)^N}{\det A}}\sum_i A_{2i}\,(A^{-1})_{1i}$$

==========calculation for 8===========

$$\int d\boldsymbol{x}\ \frac{\partial}{\partial x_1} x_1 exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right) = \int d\boldsymbol{x}\ \ (1 - x_1(A\boldsymbol{x})_1) exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right)$$

$$= \sqrt{\frac{(2\pi)^N}{\det A}} - \sum_i A_{1i}\int d\boldsymbol{x}\ \ x_1^2 exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right) = \sqrt{\frac{(2\pi)^N}{\det A}}\left(1 - (A^{-1})_{11}\sum_i A_{1i}\right)$$

=============end calculation==============

harmonic oscillator

$$-\frac{\hbar^2}{2m}\sum_i \nabla_i^2\,\psi + \frac{1}{2}m\omega^2\sum_i (x_i^2 + y_i^2 + z_i^2)\,\psi = E\psi$$

We try a linear sum of Gaussian basis function of the form

$$\psi = \psi^x\psi^y\psi^z$$

$$\psi^x = exp\left(-\frac{1}{2}\boldsymbol{x}^T A^x \boldsymbol{x} - \frac{1}{2}(\boldsymbol{x}-\boldsymbol{s}^x)^T B^x(\boldsymbol{x}-\boldsymbol{s}^x)\right)$$

Where $\boldsymbol{x}^T = (x_1, x_2, \dots . x_N)$. The energy matrix element are

$$\left\langle \psi_2^x\psi_2^y\psi_2^z\right| \textstyle\sum_i (x_i^2 + y_i^2 + z_i^2) \left|\psi_1^x\psi_1^y\psi_1^z\right\rangle =$$

$$\sum_i \Big(\langle\psi_2^x|x_i^2|\psi_1^x\rangle\langle\psi_2^y|\psi_1^y\rangle\langle\psi_2^z|\psi_1^z\rangle + \langle\psi_2^x|\psi_1^x\rangle\langle\psi_2^y|y_i^2|\psi_1^y\rangle\langle\psi_2^z|\psi_1^z\rangle$$
$$+ \langle\psi_2^x|\psi_1^x\rangle\langle\psi_2^y|\psi_1^y\rangle\langle\psi_2^z|z_i^2|\psi_1^z\rangle\Big)$$

$$\langle\psi_2^x|x_i^2|\psi_1^x\rangle = \int_{-\infty}^{\infty}\dots\int_{-\infty}^{\infty} dx_1 \dots dx_N\; exp\left(-\frac{1}{2}\boldsymbol{x}^T A_{\boldsymbol{1}}^x\boldsymbol{x} - \frac{1}{2}(\boldsymbol{x}-\boldsymbol{s}_1^x)^T B_1^x(\boldsymbol{x}-\boldsymbol{s}_1^x)\right) x_i^2\, exp\left(-\frac{1}{2}\boldsymbol{x}^T A_{\boldsymbol{2}}^x\boldsymbol{x} - \frac{1}{2}(\boldsymbol{x}-\boldsymbol{s}_2^x)^T B_2^x(\boldsymbol{x}-\boldsymbol{s}_2^x)\right)$$

$$= exp\left(-\frac{1}{2}(\boldsymbol{s}_1^x)^T B_1^x(\boldsymbol{s}_1^x) - \frac{1}{2}(\boldsymbol{s}_2^x)^T B_2^x(\boldsymbol{s}_2^x)\right)\int_{-\infty}^{\infty}\dots\int_{-\infty}^{\infty} dx_1 \dots dx_N\; x_i^2\, exp\left(-\frac{1}{2}\boldsymbol{x}^T \mathbb{A}^x\boldsymbol{x} + (B_1^x\boldsymbol{s}_1^x + B_2^x\boldsymbol{s}_2^x)\cdot\boldsymbol{x}\right)$$

$$= exp\left(-\frac{1}{2}(\boldsymbol{s}_1^x)^T B_1^x(\boldsymbol{s}_1^x) - \frac{1}{2}(\boldsymbol{s}_2^x)^T B_2^x(\boldsymbol{s}_2^x)\right)\sqrt{\frac{(2\pi)^N}{\det\mathbb{A}^x}}\, exp\left(\frac{1}{2}(B_1^x\boldsymbol{s}_1^x + B_2^x\boldsymbol{s}_2^x)^T(\mathbb{A}^x)^{-\boldsymbol{1}}(B_1^x\boldsymbol{s}_1^x + B_2^x\boldsymbol{s}_2^x)\right)$$
$$\left(\left((\mathbb{A}^x)^{-\boldsymbol{1}}(B_1^x\boldsymbol{s}_1^x + B_2^x\boldsymbol{s}_2^x)\right)_i^2 + \left((\mathbb{A}^x)^{-\boldsymbol{1}}\right)_{\boldsymbol{ii}}\right)$$

Where $\mathbb{A}^{\boldsymbol{x}} = A_{\boldsymbol{1}}^x + A_{\boldsymbol{2}}^x + B_{\boldsymbol{1}}^x + B_{\boldsymbol{2}}^x$

$$\left\langle \psi_2^x\psi_2^y\psi_2^z\right| \textstyle\sum_i (x_i^2 + y_i^2 + z_i^2) \left|\psi_1^x\psi_1^y\psi_1^z\right\rangle =$$

$$\sqrt{\frac{(2\pi)^{3N}}{\det\mathbb{A}^x\det\mathbb{A}^y\det\mathbb{A}^z}}\left(Tr\left(\mathbb{A}^{\boldsymbol{x}-\boldsymbol{1}}\right) + Tr\left(\mathbb{A}^{\boldsymbol{y}-\boldsymbol{1}}\right) + Tr\left(\mathbb{A}^{\boldsymbol{z}-\boldsymbol{1}}\right)\right)$$

=========calculation for general basis========

To calculate matrix elements we use a linear sum of Gaussian basis function of the form

$$\psi = \psi^x \psi^y \psi^z$$

$$\psi^x(\boldsymbol{x}, A^x, B^x, \boldsymbol{s}^x) = exp\left(-\frac{1}{2}\boldsymbol{x}^T A^x \boldsymbol{x} - \frac{1}{2}(\boldsymbol{x} - \boldsymbol{s}^x)^T B^x (\boldsymbol{x} - \boldsymbol{s}^x)\right)$$

for simplicity we'll drop the index x from $A, B, \boldsymbol{s}$.

=============OVERLAPE=================================

$$\langle\psi_2^x|\psi_1^x\rangle = \int d\boldsymbol{x}\, \psi^x(\boldsymbol{x}, A_2, B_2, \boldsymbol{s}_2)\psi^x(\boldsymbol{x}, A_1, B_1, \boldsymbol{s}_1)$$

$$= exp\left(-\frac{1}{2}\boldsymbol{s}_1^T B_1 \boldsymbol{s}_1 - \frac{1}{2}\boldsymbol{s}_2^T B_2 \boldsymbol{s}_2\right)\int d\boldsymbol{x}\, exp\left(-\frac{1}{2}\boldsymbol{x}^T \mathbb{A}\boldsymbol{x} + (B_1\boldsymbol{s}_1 + B_2\boldsymbol{s}_2)\cdot\boldsymbol{x}\right)$$

Where $\mathbb{A} = A_1 + A_2 + B_1 + B_2$

Using the integrals in the appendix we get

$$\langle\psi_2^x|\psi_1^x\rangle = exp\left(-\frac{1}{2}\boldsymbol{s}_1^T B_1 \boldsymbol{s}_1 - \frac{1}{2}\boldsymbol{s}_2^T B_2 \boldsymbol{s}_2\right)\sqrt{\frac{(2\pi)^N}{\det\mathbb{A}}}\; exp\left(\frac{1}{2}(B_1\boldsymbol{s}_1 + B_2\boldsymbol{s}_2)^T\mathbb{A}^{-\boldsymbol{1}}(B_1\boldsymbol{s}_1 + B_2\boldsymbol{s}_2)\right)$$

$$= \sqrt{\frac{(2\pi)^N}{\det\mathbb{A}}}\, exp\left(\frac{1}{2}\boldsymbol{s}_1^T(B_1^T\mathbb{A}^{-\boldsymbol{1}}B_1 - B_1)\boldsymbol{s}_1 - \frac{1}{2}\boldsymbol{s}_2^T(B_2^T\mathbb{A}^{-\boldsymbol{1}}B_2 - B_2)\boldsymbol{s}_2 + (B_2\boldsymbol{s}_2)^T\mathbb{A}^{-\boldsymbol{1}}(B_1\boldsymbol{s}_1)\right)$$

==

Using the integrals in the appendix we get

$$\langle\psi_2^x|x_i|\psi_1^x\rangle = \langle\psi_2^x|\psi_1^x\rangle\left(\mathbb{A}^{-\boldsymbol{1}}(B_1\boldsymbol{s}_1 + B_2\boldsymbol{s}_2)\right)_i$$

$$\left\langle\psi_2^x\middle|x_i^2\middle|\psi_1^x\right\rangle = \langle\psi_2^x|\psi_1^x\rangle\left[\left(\mathbb{A}^{-\boldsymbol{1}}(B_1\boldsymbol{s}_1 + B_2\boldsymbol{s}_2)\right)_i^2 + \mathbb{A}_{\boldsymbol{ii}}^{-\boldsymbol{1}}\right]$$

==

$$\frac{\partial}{\partial x_i}\psi^x = -\psi^x[A\boldsymbol{x} + B(\boldsymbol{x} - \boldsymbol{s})]_i$$

$$\left\langle\psi_2^x\middle|\frac{\partial}{\partial x_i}\middle|\psi_1^x\right\rangle = -\int d\boldsymbol{x}\,\psi^x(\boldsymbol{x}, A_2, B_2, \boldsymbol{s}_2)[(A_1 + B_1)\boldsymbol{x} - B_1\boldsymbol{s}_1]_i\psi^x(\boldsymbol{x}, A_1, B_1, \boldsymbol{s}_1)$$

$$= (B_1\boldsymbol{s}_1)_i\langle\psi_2^x|\psi_1^x\rangle - \sum_j^N\left(A_{ij}^1 + B_{ij}^1\right)\left\langle\psi_2^x\middle|x_j\middle|\psi_1^x\right\rangle$$

$$= \langle \psi_2^x | \psi_1^x \rangle \left[(B_1 \boldsymbol{s}_1)_i - \sum_j^N \left(A_{ij}^1 + B_{ij}^1 \right) \left(\mathbb{A}^{-\mathbf{1}} (B_1 \boldsymbol{s}_1 + B_2 \boldsymbol{s}_2) \right)_j \right]$$

$$= \langle \psi_2^x | \psi_1^x \rangle \big[B_1 \boldsymbol{s}_1 - (A_1 + B_1) \mathbb{A}^{-\mathbf{1}} (B_1 \boldsymbol{s}_1 + B_2 \boldsymbol{s}_2) \big]_i$$

====================