Angular momentum

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.

We calculate the value of the total orbital angular momentum matrix element for those basis,

$$L^2 = \left(\vec{L}_1 + \cdots \vec{L}_N\right)^2 = (L_{1x} + \cdots L_{Nx})^2 + \left(L_{1y} + \cdots L_{Ny}\right)^2 + (L_{1z} + \cdots L_{Nz})^2$$

When $L_1^z = x_1 \frac{\partial}{\partial y_1} - y_1 \frac{\partial}{\partial x_1}$ and so on. For simplicity we calculate just for two particle

$$(L_{1z} + L_{2z})^2 = L_{1z}^2 + L_{2z}^2 + 2L_{1z}L_{2z}$$

$$= \left(x_1 \frac{\partial}{\partial y_1} - y_1 \frac{\partial}{\partial x_1}\right)^2 + \left(x_2 \frac{\partial}{\partial y_2} - y_2 \frac{\partial}{\partial x_2}\right)^2 + 2\left(x_1 \frac{\partial}{\partial y_1} - y_1 \frac{\partial}{\partial x_1}\right)\left(x_2 \frac{\partial}{\partial y_2} - y_2 \frac{\partial}{\partial x_2}\right)$$

$$= \left(x_1^2 \frac{\partial^2}{\partial y_1^2} - x_1 \frac{\partial}{\partial y_1} y_1 \frac{\partial}{\partial x_1} - y_1 \frac{\partial}{\partial x_1} x_1 \frac{\partial}{\partial y_1} + y_1^2 \frac{\partial^2}{\partial x_1^2}\right)$$

$$+ \left(x_2^2 \frac{\partial^2}{\partial y_2^2} - x_2 \frac{\partial}{\partial y_2} y_2 \frac{\partial}{\partial x_2} - y_2 \frac{\partial}{\partial x_2} x_2 \frac{\partial}{\partial y_2} + y_2^2 \frac{\partial^2}{\partial x_2^2}\right)$$

$$+2\left(x_1 \frac{\partial}{\partial y_1} x_2 \frac{\partial}{\partial y_2} - x_1 \frac{\partial}{\partial y_1} y_2 \frac{\partial}{\partial x_2} - y_1 \frac{\partial}{\partial x_1} x_2 \frac{\partial}{\partial y_2} + y_1 \frac{\partial}{\partial x_1} y_2 \frac{\partial}{\partial x_2}\right)$$

There are four kind of terms that we need to calculate…

$$\left\langle \psi'^x \psi'^y \psi'^z \middle| x_1^2 \frac{\partial^2}{\partial y_1^2} \middle| \psi^x \psi^y \psi^z \right\rangle = \langle \psi'^x | x_1^2 | \psi^x \rangle \left\langle \psi'^y \middle| \frac{\partial^2}{\partial y_1^2} \middle| \psi^y \right\rangle \langle \psi'^z | \psi^z \rangle$$

$$\left\langle \psi'^x \psi'^y \psi'^z \middle| x_1 \frac{\partial}{\partial y_1} y_1 \frac{\partial}{\partial x_1} \middle| \psi^x \psi^y \psi^z \right\rangle = \left\langle \psi'^x \middle| x_1 \frac{\partial}{\partial x_1} \middle| \psi^x \right\rangle \left\langle \psi'^y \middle| \frac{\partial}{\partial y_1} y_1 \middle| \psi^y \right\rangle \langle \psi'^z | \psi^z \rangle$$

$$\left\langle \psi'^x \psi'^y \psi'^z \middle| x_1 \frac{\partial}{\partial y_1} x_2 \frac{\partial}{\partial y_2} \middle| \psi^x \psi^y \psi^z \right\rangle = \langle \psi'^x | x_1 x_2 | \psi^x \rangle \left\langle \psi'^y \middle| \frac{\partial}{\partial y_1} \frac{\partial}{\partial y_2} \middle| \psi^y \right\rangle \langle \psi'^z | \psi^z \rangle$$

$$\left\langle \psi'^x \psi'^y \psi'^z \middle| x_1 \frac{\partial}{\partial y_1} y_2 \frac{\partial}{\partial x_2} \middle| \psi^x \psi^y \psi^z \right\rangle = \left\langle \psi'^x \middle| x_1 \frac{\partial}{\partial x_2} \middle| \psi^x \right\rangle \left\langle \psi'^y \middle| y_2 \frac{\partial}{\partial y_1} \middle| \psi^y \right\rangle \langle \psi'^z | \psi^z \rangle$$

So we need the analytical expression for 8 matrix elements, 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) $\langle\psi'^x|x_1x_2|\psi^x\rangle = \sqrt{\frac{(2\pi)^N}{\det\mathbb{A}_x}}(\mathbb{A}_x^{-1})_{21}$

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

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

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

$$\sum_k^N A_{ik}'^xA_{ik}^x\,(\mathbb{A}_x^{-1})_{kk} = \sum_k^N\sum_{ij}A_{ki}'^xA_{kj}^x\,(\mathbb{A}_x^{-1})_{ij}$$

Now

$$\langle\psi'^x\psi'^y\psi'^z|(L_{1z}+L_{2z})^2|\psi^x\psi^y\psi^z\rangle = \sqrt{\frac{(2\pi)^{3N}}{\det\mathbb{A}_x\det\mathbb{A}_y\det\mathbb{A}_z}}\times$$

$$+(\mathbb{A}_x^{-1})_{11}\left(-A_{11}^y + \sum_{ij}A_{1i}^yA_{1j}^y\left(\mathbb{A}_y^{-1}\right)_{ij}\right) + \sum_i A_{1i}^x\,(\mathbb{A}_x^{-1})_{1i}\left(1 - \left(\mathbb{A}_y^{-1}\right)_{11}\sum_i A_{1i}^y\right)$$

$$+\sum_i A_{1i}^y\left(\mathbb{A}_y^{-1}\right)_{1i}\left(1 - (\mathbb{A}_x^{-1})_{11}\sum_i A_{1i}^x\right) + \left(\mathbb{A}_y^{-1}\right)_{11}\left(-A_{11}^x + \sum_{ij}A_{1i}^xA_{1j}^x\,(\mathbb{A}_x^{-1})_{ij}\right)$$

$$+(\mathbb{A}_x^{-1})_{22}\left(-A_{22}^y + \sum_{ij}A_{2i}^yA_{2j}^y\left(\mathbb{A}_y^{-1}\right)_{ij}\right) + \sum_i A_{2i}^x\,(\mathbb{A}_x^{-1})_{1i}\left(1 - \left(\mathbb{A}_y^{-1}\right)_{22}\sum_i A_{2i}^y\right)$$

$$+\sum_i A^y_{2i}\left(\mathbb{A}_y^{-1}\right)_{2i}\left(1-(\mathbb{A}_x^{-1})_{22}\sum_i A^x_{2i}\right)+\left(\mathbb{A}_y^{-1}\right)_{22}\left(-A^x_{22}+\sum_{ij}A^x_{2i}A^x_{2j}\,(\mathbb{A}_x^{-1})_{ij}\right)$$

$$+2(\mathbb{A}_x^{-1})_{21}\left(-A^y_{21}+\sum_{ij}A^y_{2i}A^y_{1j}\left(\mathbb{A}_y^{-1}\right)_{ij}\right)-2\sum_i A^x_{2i}\,(\mathbb{A}_x^{-1})_{1i}\sum_i A^y_{1i}\left(\mathbb{A}_y^{-1}\right)_{2i}$$

$$-2\sum_i A^x_{1i}\,(\mathbb{A}_x^{-1})_{2i}\sum_i A^y_{2i}\left(\mathbb{A}_y^{-1}\right)_{1i}+2\left(\mathbb{A}_y^{-1}\right)_{21}\left(-A^x_{21}+\sum_{ij}A^x_{2i}A^x_{1j}\,(\mathbb{A}_x^{-1})_{ij}\right)$$

$$\langle\psi'^x\psi'^y\psi'^z|(L_{1z}+\cdots L_{Nz})^2|\psi^x\psi^y\psi^z\rangle=\sqrt{\frac{(2\pi)^{3N}}{\det\mathbb{A}_x\det\mathbb{A}_y\det\mathbb{A}_z}}\times$$

$$\sum_{k=1}^{N}$$

$$+(\mathbb{A}_x^{-1})_{kk}\left(-A^y_{kk}+\sum_{ij}A^y_{ki}A^y_{kj}\left(\mathbb{A}_y^{-1}\right)_{ij}\right)+\sum_i A^x_{ki}\,(\mathbb{A}_x^{-1})_{ki}\left(1-\left(\mathbb{A}_y^{-1}\right)_{kk}\sum_i A^y_{1i}\right)$$

$$+\sum_i A^y_{ki}\left(\mathbb{A}_y^{-1}\right)_{ki}\left(1-(\mathbb{A}_x^{-1})_{kk}\sum_i A^x_{ki}\right)+\left(\mathbb{A}_y^{-1}\right)_{kk}\left(-A^x_{kk}+\sum_{ij}A^x_{ki}A^x_{kj}\,(\mathbb{A}_x^{-1})_{ij}\right)$$

$$\sum_{n,m=1}^{N}$$

$$+(\mathbb{A}_x^{-1})_{nm}\left(-A^y_{nm}+\sum_{ij}A^y_{ni}A^y_{mj}\left(\mathbb{A}_y^{-1}\right)_{ij}\right)-\sum_i A^x_{ni}\,(\mathbb{A}_x^{-1})_{mi}\sum_i A^y_{ni}\left(\mathbb{A}_y^{-1}\right)_{mi}$$

$$-\sum_i A^x_{mi}\,(\mathbb{A}_x^{-1})_{ni}\sum_i A^y_{mi}\left(\mathbb{A}_y^{-1}\right)_{ni}+\left(\mathbb{A}_y^{-1}\right)_{21}\left(-A^x_{nm}+\sum_{ij}A^x_{ni}A^x_{mj}\,(\mathbb{A}_x^{-1})_{ij}\right)$$

$$\langle \psi'^x \psi'^y \psi'^z | (L_{1z} + \cdots L_{Nz})^2 | \psi^x \psi^y \psi^z \rangle = \sqrt{\frac{(2\pi)^{3N}}{\det \mathbb{A}_x \det \mathbb{A}_y \det \mathbb{A}_z}} \times$$

$$\sum_{k=1}^{N}$$

$$-C_{kk} B_{kk} + C_{kk} \sum_{ij} B_{ki} B_{kj} D_{ij} + \sum_i A_{ki} C_{ki} - \sum_i A_{ki} C_{ki} D_{kk} \sum_i B_{ki}$$

$$+ \sum_i B_{ki} D_{ki} - \sum_i B_{ki} D_{ki} C_{kk} \sum_i A_{ki} - D_{kk} A_{kk} + D_{kk} \sum_{ij} A_{ki} A_{kj} C_{ij}$$

$$\sum_{n,m=1}^{N}$$

$$-C_{nm} B_{mn} + C_{nm} \sum_{ij} B_{ni} B_{mj} D_{ij} - \sum_i A_{ni} C_{mi} \sum_i B_{ni} D_{mi}$$

$$- \sum_i A_{mi} C_{ni} \sum_i B_{mi} D_{ni} - D_{mn} A_{nm} + D_{mn} \sum_{ij} A_{ni} A_{mj} C_{ij}$$

$$\langle \psi'^x \psi'^y \psi'^z | (L_{1z} + \cdots L_{Nz})^2 | \psi^x \psi^y \psi^z \rangle = \sqrt{\frac{(2\pi)^{3N}}{\det \mathbb{A}_x \det \mathbb{A}_y \det \mathbb{A}_z}} \times$$

$$\sum_{k=1}^{N} C_{kk} \left(-B_{kk} + (BDB)_{kk} - (BD)_{kk} \sum_i A_{ki} \right) + D_{kk} \left(-A_{kk} + (ACA)_{kk} - (AC)_{kk} \sum_i B_{ki} \right)$$

$$+tr(BD) + tr(AC) + tr(CBDB) + tr(DACA) - tr(BC) - tr(AD) - 2tr(ACBD)$$

$$A = A^x, \qquad B = A^y, \quad C = \mathbb{A}_x^{-1}, \quad D = \mathbb{A}_y^{-1}$$

APPENDIX

=======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 appendix==============