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

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

Where

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

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

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

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

We used $\frac{1}{2}\boldsymbol{x}^{\boldsymbol{T}} B\boldsymbol{s} + \frac{1}{2}\boldsymbol{s}^{\boldsymbol{T}} B\boldsymbol{x} = (B\boldsymbol{s})\cdot\boldsymbol{x}$ (see * below)

So we can define the basis function as

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

When $A = A + B$, $\boldsymbol{b} = B\boldsymbol{s}$, $C = exp\left(-\frac{1}{2}\boldsymbol{s}^{\boldsymbol{T}} B\boldsymbol{s}\right)$

And calculate all matrix element for this basis.

We denote,

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

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

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

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

Using the integrals in the appendix where $\mathbb{A} = A_1 + A_2$ $\mathfrak{b} = \boldsymbol{b}_1 + \boldsymbol{b}_2$

===================Magnetic ME====================

$$\langle\psi_2^x|x_i x_j|\psi_1^x\rangle = \int d\boldsymbol{x}\, x_i x_j exp\left(-\frac{1}{2}\boldsymbol{x}^T \mathbb{A}\boldsymbol{x} + \mathfrak{b}\cdot\boldsymbol{x}\right)$$

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

$$= \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} \frac{\partial}{\partial \mathfrak{b}_i} (\mathbb{A}^{-1}\mathfrak{b})_j exp\left(\frac{1}{2} \mathfrak{b}^T \mathbb{A}^{-1} \mathfrak{b}\right)$$

$$= \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} exp\left(\frac{1}{2} \mathfrak{b}^T \mathbb{A}^{-1} \mathfrak{b}\right) \left(\mathbb{A}_{ij}^{-1} + (\mathbb{A}^{-1}\mathfrak{b})_i (\mathbb{A}^{-1}\mathfrak{b})_j\right)$$

==

$$\langle \psi_2^x | x_i^2 | \psi_1^x \rangle = \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} exp\left(\frac{1}{2} \mathfrak{b}^T \mathbb{A}^{-1} \mathfrak{b}\right) \left(\mathbb{A}_{ii}^{-1} + (\mathbb{A}^{-1}\mathfrak{b})_i^2\right)$$

Just substitute $i = j$ in $\langle \psi_2^x | x_i x_j | \psi_1^x \rangle$.

If we sum over the particles (sum over i) we get

$$\sum_i \left(\mathbb{A}_{ii}^{-1} + (\mathbb{A}^{-1}\mathfrak{b})_i^2\right) = tr(\mathbb{A}^{-1}) + \sum_i (\mathbb{A}^{-1}\mathfrak{b})_i^2$$

==

$$\left\langle \psi_2^x \middle| \left(x_i - x_j\right)^2 \middle| \psi_1^x \right\rangle = \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} exp\left(\frac{1}{2} \mathfrak{b}^T \mathbb{A}^{-1} \mathfrak{b}\right) \left(\mathbb{A}_{ii}^{-1} + \mathbb{A}_{jj}^{-1} - 2\mathbb{A}_{ij}^{-1}\right)$$

$$+ \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} exp\left(\frac{1}{2} \mathfrak{b}^T \mathbb{A}^{-1} \mathfrak{b}\right) \left((\mathbb{A}^{-1}\mathfrak{b})_i^2 + (\mathbb{A}^{-1}\mathfrak{b})_j^2 - 2(\mathbb{A}^{-1}\mathfrak{b})_i (\mathbb{A}^{-1}\mathfrak{b})_j\right)$$

===================Kinetic Energy===============

$$\left\langle \psi_2^x \middle| \frac{\partial^2}{\partial x_i^2} \middle| \psi_1^x \right\rangle = \int d\boldsymbol{x} exp\left(-\frac{1}{2} \boldsymbol{x}^T A_1 \boldsymbol{x} + \boldsymbol{b}_1 \cdot \boldsymbol{x}\right) \frac{\partial^2}{\partial x_i^2} exp\left(-\frac{1}{2} \boldsymbol{x}^T A_2 \boldsymbol{x} + \boldsymbol{b}_2 \cdot \boldsymbol{x}\right)$$

$$= -\int d\boldsymbol{x} \left(\frac{\partial}{\partial x_i} exp\left(-\frac{1}{2} \boldsymbol{x}^T A_1 \boldsymbol{x} + \boldsymbol{b}_1 \cdot \boldsymbol{x}\right)\right) \left(\frac{\partial}{\partial x_i} exp\left(-\frac{1}{2} \boldsymbol{x}^T A_2 \boldsymbol{x} + \boldsymbol{b}_2 \cdot \boldsymbol{x}\right)\right)$$

$$= -\int d\boldsymbol{x} \, (-A_1 \boldsymbol{x} + \boldsymbol{b}_1)_i (-A_2 \boldsymbol{x} + \boldsymbol{b}_2)_i exp\left(-\frac{1}{2} \boldsymbol{x}^T \mathbb{A} \boldsymbol{x} + \mathfrak{b} \cdot \boldsymbol{x}\right)$$

$$= -\sum_{nm} A_{in}^1 A_{im}^2 \int d\boldsymbol{x} \, x_n x_m exp\left(-\frac{1}{2} \boldsymbol{x}^T \mathbb{A} \boldsymbol{x} + \mathfrak{b} \cdot \boldsymbol{x}\right)$$

$$+ \left((\boldsymbol{b}_2)_i \sum_n A_{in}^1 + (\boldsymbol{b}_1)_i \sum_n A_{in}^2\right) \int d\boldsymbol{x} \, x_n exp\left(-\frac{1}{2} \boldsymbol{x}^T \mathbb{A} \boldsymbol{x} + \mathfrak{b} \cdot \boldsymbol{x}\right)$$

$$-(\boldsymbol{b}_1)_i (\boldsymbol{b}_2)_i \int d\boldsymbol{x} \, exp\left(-\frac{1}{2} \boldsymbol{x}^T \mathbb{A} \boldsymbol{x} + \mathfrak{b} \cdot \boldsymbol{x}\right)$$

$$= -\sum_{nm} A^1_{in} A^2_{im} \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} (\mathbb{A}^{-1}_{nm} + (\mathbb{A}^{-1}\mathfrak{b})_n (\mathbb{A}^{-1}\mathfrak{b})_m) exp\left(\frac{1}{2}\mathfrak{b}^T \mathbb{A}^{-1}\mathfrak{b}\right)$$

$$+\left((\boldsymbol{b}_2)_i \sum_n A^1_{in} + (\boldsymbol{b}_1)_i \sum_n A^2_{in}\right) \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} (\mathbb{A}^{-1}\mathfrak{b})_n exp\left(\frac{1}{2}\mathfrak{b}^T \mathbb{A}^{-1}\mathfrak{b}\right)$$

$$-(\boldsymbol{b}_1)_i (\boldsymbol{b}_2)_i \sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} exp\left(\frac{1}{2}\mathfrak{b}^T \mathbb{A}^{-1}\mathfrak{b}\right)$$

$$= -\sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} exp\left(\frac{1}{2}\mathfrak{b}^T \mathbb{A}^{-1}\mathfrak{b}\right) \sum_{nm} A^1_{in} A^2_{im}\, \mathbb{A}^{-1}_{nm}$$

$$+\sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} exp\left(\frac{1}{2}\mathfrak{b}^T \mathbb{A}^{-1}\mathfrak{b}\right) \times$$

$$\left(\left((\boldsymbol{b}_2)_i \sum_n A^1_{in} + (\boldsymbol{b}_1)_i \sum_n A^2_{in}\right) (\mathbb{A}^{-1}\mathfrak{b})_n - \sum_{nm} A^1_{in} A^2_{im} (\mathbb{A}^{-1}\mathfrak{b})_n (\mathbb{A}^{-1}\mathfrak{b})_m - (\boldsymbol{b}_1)_i (\boldsymbol{b}_2)_i\right)$$

If we sum over the particles (sum over i) we get

$$= -\sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} exp\left(\frac{1}{2}\mathfrak{b}^T \mathbb{A}^{-1}\mathfrak{b}\right) tr(A_1 \mathbb{A}^{-1} A_2)$$

$$+\sqrt{\frac{(2\pi)^N}{\det \mathbb{A}}} exp\left(\frac{1}{2}\mathfrak{b}^T \mathbb{A}^{-1}\mathfrak{b}\right) \left(\boldsymbol{b}_2^{\boldsymbol{T}} A_1 \mathbb{A}^{-1}\mathfrak{b} + \boldsymbol{b}_1^{\boldsymbol{T}} A_2 \mathbb{A}^{-1}\mathfrak{b} - (A_1 \mathbb{A}^{-1}\mathfrak{b}) \cdot (A_2 \mathbb{A}^{-1}\mathfrak{b}) - \boldsymbol{b}_1 \cdot \boldsymbol{b}_2\right)$$

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It can be prove that

$$\boldsymbol{b}_2^{\boldsymbol{T}} A_1 \mathbb{A}^{-1}\mathfrak{b} + \boldsymbol{b}_1^{\boldsymbol{T}} A_2 \mathbb{A}^{-1}\mathfrak{b} - (A_1 \mathbb{A}^{-1}\mathfrak{b}) \cdot (A_2 \mathbb{A}^{-1}\mathfrak{b}) - \boldsymbol{b}_1 \cdot \boldsymbol{b}_2 =$$

$$(A_2 \mathbb{A}^{-1}\boldsymbol{b}_1 - \boldsymbol{A}_1 \mathbb{A}^{-1}\boldsymbol{b}_2) \cdot (A_2 \mathbb{A}^{-1}\boldsymbol{b}_1 - \boldsymbol{A}_1 \mathbb{A}^{-1}\boldsymbol{b}_2)$$

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========================Two body energy============================

The 2-body potential is $\sum_{i<j} V^x_{ij} V^y_{ij} V^z_{ij}$ where $V^x_{ij} = e^{-a x^2_{ij}}$ where $x_{ij} = x_i - x_j$

The matrix element that we need to calculate is $\sum_{i<j} \langle \psi^x_2 | V^x_{ij} | \psi^x_1 \rangle \langle \psi^y_2 | V^y_{ij} | \psi^y_1 \rangle \langle \psi^z_2 | V^z_{ij} | \psi^z_1 \rangle$

$$\langle \psi^x_2 | V^x_{ij} | \psi^x_1 \rangle = \int d\boldsymbol{x}\, exp(-a x^2_{ij}) exp\left(-\frac{1}{2}\boldsymbol{x}^T \mathbb{A}\boldsymbol{x} + \mathfrak{b} \cdot \boldsymbol{x}\right)$$

Where $\mathbb{A} = A_1 + A_2$ $\quad \mathfrak{b} = \boldsymbol{b}_1 + \boldsymbol{b}_2$ and $\boldsymbol{x}^T = (x_1, x_2, \dots . x_N)$.

Write the potential as $V_{ij}^x = \int dy e^{-ay^2}\delta(y - x_{ij})$ and first we calculate the integral,

$$\langle\psi_2^x|\delta(y - x_{ij})|\psi_1^x\rangle = \int d\boldsymbol{x}\,\delta(y - x_{ij}) exp\left(-\frac{1}{2}\boldsymbol{x}^T\mathbb{A}\boldsymbol{x} + \mathfrak{b}\cdot\boldsymbol{x}\right)$$

Where $x_{ij} = x_i - x_j$ but in the general case $x_{ij} = \boldsymbol{C}^{ij}\cdot\boldsymbol{x}$.

Using

$$\delta(y - \boldsymbol{C}^{ij}\cdot\boldsymbol{x}) = \int \frac{dk}{2\pi} exp\left(ik(y - \boldsymbol{C}^{ij}\cdot\boldsymbol{x})\right)$$

We get

$$= \int \frac{dk}{2\pi} exp(iky) \int d\boldsymbol{x}\, exp\left(-\frac{1}{2}\boldsymbol{x}^T\mathbb{A}\boldsymbol{x} + (\mathfrak{b} - ik\boldsymbol{C}^{ij})\cdot\boldsymbol{x}\right)$$

$$= \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}}\int\frac{dk}{2\pi} exp(iky)\, exp\left(\frac{1}{2}(\mathfrak{b} - ik\boldsymbol{C}^{ij})^T\mathbb{A}^{-1}(\mathfrak{b} - ik\boldsymbol{C}^{ij})\right)$$

$$= \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}} exp\left(\frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\mathfrak{b}\right)$$

$$\times\int\frac{dk}{2\pi} exp\left(-\frac{1}{2}(\boldsymbol{C}^{ij})^T\mathbb{A}^{-1}\boldsymbol{C}^{ij}k^2 + ik\left(y - \frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\boldsymbol{C}^{ij} - \frac{1}{2}(\boldsymbol{C}^{ij})^T\mathbb{A}^{-1}\mathfrak{b}\right)\right)$$

Denote $s = (\boldsymbol{C}^{ij})^T\mathbb{A}^{-1}\boldsymbol{C}^{ij}$, $r = \frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\boldsymbol{C}^{ij} + \frac{1}{2}(\boldsymbol{C}^{ij})^T\mathbb{A}^{-1}\mathfrak{b} = \mathfrak{b}^T\mathbb{A}^{-1}\boldsymbol{C}^{ij}$ (see * below)

we need to calculate

$$\sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}} exp\left(\frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\mathfrak{b}\right)\int\frac{dk}{2\pi} exp\left(-\frac{1}{2}sk^2 + ik(y - r)\right)$$

Using $\int dx e^{-\frac{1}{2}ax^2 + bx} = \sqrt{\frac{2\pi}{a}}e^{\frac{b^2}{2a}}$ we get

$$= \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}} exp\left(\frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\mathfrak{b}\right)\frac{1}{\sqrt{2\pi s}}\exp\left(-\frac{(y-r)^2}{2s}\right)$$

Now

$$\langle\psi_2^x|V_{ij}^x|\psi_1^x\rangle = \langle\psi_2^x|\int dy e^{-ay^2}\delta(y - x_{ij})\,|\psi_1^x\rangle = \int dy e^{-ay^2}\langle\psi_2^x|\delta(y - x_{ij})|\psi_1^x\rangle$$

$$= \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}} exp\left(\frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\mathfrak{b}\right)\frac{1}{\sqrt{2\pi s}}\int dy e^{-ay^2}\exp\left(-\frac{(y-r)^2}{2s}\right)$$

$$= \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}}\, exp\left(\frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\mathfrak{b}\right)\exp\left(-\frac{r^2}{2s}\right)\frac{1}{\sqrt{2\pi s}}\int dy \exp\left(-\frac{1}{2}\left(\frac{1}{s}+2a\right)y^2+\frac{r}{s}y\right)$$

$$= \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}}\, exp\left(\frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\mathfrak{b}\right)\exp\left(-\frac{r^2}{2s}\right)\frac{1}{\sqrt{2\pi s}}\sqrt{\frac{2\pi}{\left(\frac{1}{s}+2a\right)}}\exp\left(\frac{\frac{r^2}{s^2}}{2\left(\frac{1}{s}+2a\right)}\right)$$

Finally

$$\langle\psi_2^x|V_{ij}^x|\psi_1^x\rangle = \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}}\sqrt{\frac{1}{1+2as}}\, exp\left(\frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\mathfrak{b}\right)\exp\left(-\frac{ar^2}{1+2as}\right)$$

When

$r = \mathfrak{b}^T\mathbb{A}^{-1}\boldsymbol{C}^{ij}$

$s = \left(\boldsymbol{C}^{ij}\right)^T\mathbb{A}^{-1}\boldsymbol{C}^{ij}$

===========================Three body energy========================

The 2-body potential is $\sum_{cyc}\sum_{i<j<k} V_{ijk}^x V_{ijk}^y V_{ijk}^z$ Where $V_{ijk}^x = e^{-a\left(x_{ik}^2+x_{jk}^2\right)}$, $x_{ij} \equiv x_i - x_j$

$$\langle\psi_2^x|V_{ijk}^x|\psi_1^x\rangle = \int d\boldsymbol{x}\, exp\left(-a\left(x_{ik}^2+x_{jk}^2\right)\right) exp\left(-\frac{1}{2}\boldsymbol{x}^T\mathbb{A}\boldsymbol{x}+\mathfrak{b}\cdot\boldsymbol{x}\right)$$

Where $\mathbb{A} = A_1 + A_2$ $\mathfrak{b} = \boldsymbol{b}_1 + \boldsymbol{b}_2$ and $\boldsymbol{x}^T = (x_1, x_2, \ldots .x_N)$.

Write the potential as $V_{ijk}^x = \int dy_1 dy_2 e^{-a\left(y_1^2+y_2^2\right)}\delta(y_1 - x_{ik})\delta\left(y_2 - x_{jk}\right)$ and first we calculate the integral,

$$\langle\psi_2^x|\delta(y_1 - x_{ik})\delta\left(y_2 - x_{jk}\right)|\psi_1^x\rangle = \int d\boldsymbol{x}\,\delta(y_1 - x_{ik})\delta\left(y_2 - x_{jk}\right) exp\left(-\frac{1}{2}\boldsymbol{x}^T\mathbb{A}\boldsymbol{x}+\mathfrak{b}\cdot\boldsymbol{x}\right)$$

Where $x_{ij} = x_i - x_j$ but in the general case $x_{ij} = \boldsymbol{C}^{ij}\cdot\boldsymbol{x}$.

Using

$$\delta\left(y - \boldsymbol{C}^{ij}\cdot\boldsymbol{x}\right) = \int\frac{dk}{2\pi} exp\left(ik\left(y - \boldsymbol{C}^{ij}\cdot\boldsymbol{x}\right)\right)$$

We get

$$= \int\frac{dk_1}{2\pi}\frac{dk_2}{2\pi}\int d\boldsymbol{x}\, exp\left(ik_1\left(y_1 - \boldsymbol{C}^{ik}\cdot\boldsymbol{x}\right)\right) exp\left(ik_2\left(y_2 - \boldsymbol{C}^{jk}\cdot\boldsymbol{x}\right)\right) exp\left(-\frac{1}{2}\boldsymbol{x}^T\mathbb{A}\boldsymbol{x}+\mathfrak{b}\cdot\boldsymbol{x}\right)$$

$$= \int\frac{dk_1}{2\pi}\frac{dk_2}{2\pi} exp(ik_1y_1)\, exp(ik_2y_2)\int d\boldsymbol{x}\, exp\left(-\frac{1}{2}\boldsymbol{x}^T\mathbb{A}\boldsymbol{x}+\left(\mathfrak{b} - ik_1\boldsymbol{C}^{ik} - ik_2\boldsymbol{C}^{jk}\right)\cdot\boldsymbol{x}\right)$$

$$= \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}} \int \frac{dk_1}{2\pi}\frac{dk_2}{2\pi} exp(ik_1 y_1)\, exp(ik_2 y_2)$$

$$\times\, exp\left(\frac{1}{2}\left(\mathfrak{b} - ik_1\boldsymbol{C}^{ik} - ik_2\boldsymbol{C}^{jk}\right)^{\boldsymbol{T}} \mathbb{A}^{-1}\left(\mathfrak{b} - ik_1\boldsymbol{C}^{ik} - ik_2\boldsymbol{C}^{jk}\right)\right)$$

$$= \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}}\, exp\left(\frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\mathfrak{b}\right) \int \frac{dk_1}{2\pi}\frac{dk_2}{2\pi}$$

$$\times\, exp\left(ik_1\left(y_1 - \frac{1}{2}\left(\boldsymbol{C}^{ik}\right)^{\boldsymbol{T}}\mathbb{A}^{-1}\mathfrak{b} - \frac{1}{2}\mathfrak{b}^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{ik}\right) + ik_2\left(y_2 - \frac{1}{2}\left(\boldsymbol{C}^{jk}\right)^{\boldsymbol{T}}\mathbb{A}^{-1}\mathfrak{b} - \frac{1}{2}\mathfrak{b}^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{jk}\right)\right)$$

$$\times\, exp\left(-\frac{1}{2}\left(k_1\boldsymbol{C}^{ik} + k_2\boldsymbol{C}^{jk}\right)^{\boldsymbol{T}}\mathbb{A}^{-1}\left(k_1\boldsymbol{C}^{ik} + k_2\boldsymbol{C}^{jk}\right)\right)$$

Define $\quad \boldsymbol{k} = \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} \quad \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \quad \boldsymbol{r} = \begin{pmatrix} \frac{1}{2}\left(\boldsymbol{C}^{ik}\right)^{\boldsymbol{T}}\mathbb{A}^{-1}\mathfrak{b} + \frac{1}{2}\mathfrak{b}^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{ik} \\ \frac{1}{2}\left(\boldsymbol{C}^{jk}\right)^{\boldsymbol{T}}\mathbb{A}^{-1}\mathfrak{b} + \frac{1}{2}\mathfrak{b}^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{jk} \end{pmatrix} \underbrace{=}_{see*} \begin{pmatrix} \mathfrak{b}^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{ik} \\ \mathfrak{b}^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{jk} \end{pmatrix}$

$$S = \begin{pmatrix} \left(\boldsymbol{C}^{ik}\right)^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{ik} & \left(\boldsymbol{C}^{ik}\right)^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{jk} \\ \left(\boldsymbol{C}^{jk}\right)^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{ik} & \left(\boldsymbol{C}^{jk}\right)^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{jk} \end{pmatrix}$$

We get

$$\langle \psi_2^x | \delta(y_1 - x_{ik})\delta(y_2 - x_{jk}) | \psi_1^x \rangle$$

$$= \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}}\, exp\left(\frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\mathfrak{b}\right)\frac{1}{(2\pi)^2}\int d\boldsymbol{k}\, exp\left(-\frac{1}{2}\boldsymbol{k}^{\boldsymbol{T}}S\boldsymbol{k} + i(\boldsymbol{y} - \boldsymbol{r})\cdot\boldsymbol{k}\right)$$

$$= \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}}\, exp\left(\frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\mathfrak{b}\right)\sqrt{\frac{1}{(2\pi)^2\det S}}\, exp\left(-\frac{1}{2}(\boldsymbol{y} - \boldsymbol{r})^T S^{-1}(\boldsymbol{y} - \boldsymbol{r})\right)$$

Now

$$\langle \psi_2^x | V_{ijk}^x | \psi_1^x \rangle = \langle \psi_2^x | \int dy_1 dy_2 e^{-a\left(y_1^2 + y_2^2\right)}\delta(y_1 - x_{ik})\delta(y_2 - x_{jk}) | \psi_1^x \rangle$$

$$= \int dy_1 dy_2 e^{-a\left(y_1^2 + y_2^2\right)} \langle \psi_2^x | \delta(y_1 - x_{ik})\delta(y_2 - x_{jk}) | \psi_1^x \rangle$$

$$= \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}}\, exp\left(\frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\mathfrak{b}\right)\sqrt{\frac{1}{(2\pi)^2\det S}}\int d\boldsymbol{y}\, exp\left(-\frac{1}{2}(\boldsymbol{y} - \boldsymbol{r})^T S^{-1}(\boldsymbol{y} - \boldsymbol{r}) - a\boldsymbol{y}^T\boldsymbol{y}\right)$$

$$= \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}}\, exp\left(\frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\mathfrak{b}\right)\sqrt{\frac{1}{(2\pi)^2\det S}}\; exp\left(-\frac{1}{2}\boldsymbol{r}^T S^{-1}\boldsymbol{r}\right)$$

$$\times \int d\boldsymbol{y}\, exp\left(-\frac{1}{2}\boldsymbol{y}^T(S^{-1}+2aI)\boldsymbol{y}+(S^{-1}\boldsymbol{r})\cdot\boldsymbol{y}\right)$$

We used $\frac{1}{2}\boldsymbol{r}^T S^{-1}\boldsymbol{y}+\frac{1}{2}\boldsymbol{y}^T S^{-1}\boldsymbol{r}=(S^{-1}\boldsymbol{r})\cdot\boldsymbol{y}$ ***(****see * below)*

$$\int d\boldsymbol{y}\, exp\left(-\frac{1}{2}\boldsymbol{y}^T(S^{-1}+2aI)\boldsymbol{y}+(S^{-1}\boldsymbol{r})\cdot\boldsymbol{y}\right)$$

$$=\sqrt{\frac{(2\pi)^2}{\det(S^{-1}+2aI)}}\, exp\left(\frac{1}{2}(S^{-1}\boldsymbol{r})^T(S^{-1}+2aI)^{-1}(S^{-1}\boldsymbol{r})\right)$$

Finally

$$\langle\psi_2^x|V_{ijk}^x|\psi_1^x\rangle=\sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}}}\sqrt{\frac{1}{\det(2aS+I)}}\, exp\left(\frac{1}{2}\mathfrak{b}^T\mathbb{A}^{-1}\mathfrak{b}\right)$$

$$\times\, exp\left(\frac{1}{2}(S^{-1}\boldsymbol{r})^T(S^{-1}+2aI)^{-1}(S^{-1}\boldsymbol{r})-\frac{1}{2}\boldsymbol{r}^T S^{-1}\boldsymbol{r}\right)$$

Where

$$\boldsymbol{r}=\begin{pmatrix}\mathfrak{b}^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{ik}\\ \mathfrak{b}^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{jk}\end{pmatrix}$$

$$S=\begin{pmatrix}\left(\boldsymbol{C}^{ik}\right)^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{ik} & \left(\boldsymbol{C}^{ik}\right)^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{jk}\\ \left(\boldsymbol{C}^{jk}\right)^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{ik} & \left(\boldsymbol{C}^{jk}\right)^{\boldsymbol{T}}\mathbb{A}^{-1}\boldsymbol{C}^{jk}\end{pmatrix}$$

$$I=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

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*

If A symmetric matrix then $\frac{1}{2}\boldsymbol{a}^{\boldsymbol{T}}A\boldsymbol{b}+\frac{1}{2}\boldsymbol{b}^{\boldsymbol{T}}A\boldsymbol{a}=(A\boldsymbol{a})\cdot\boldsymbol{b}=(A\boldsymbol{b})\cdot\boldsymbol{a}$

$$\boldsymbol{a}^T A\boldsymbol{b}=\sum_{ij}a_iA_{ij}\,b_j=\sum_{ij}a_jA_{ji}\,b_i=\sum_{ij}b_iA_{ij}\,a_j=\boldsymbol{b}^T A\boldsymbol{a}$$

$$\frac{1}{2}\boldsymbol{a}^{\boldsymbol{T}}A\boldsymbol{b}+\frac{1}{2}\boldsymbol{b}^{\boldsymbol{T}}A\boldsymbol{a}=\boldsymbol{a}^T A\boldsymbol{b}=\sum_{ij}A_{ij}a_i\,b_j=\sum_{ij}A_{ij}a_j\,b_i=(A\boldsymbol{a})\cdot\boldsymbol{b}$$

==

$$V = \sum_{k,l} C_{kl} \sum_{i<j} O_{ij}^{k}\, exp\left(-a_{kl}\boldsymbol{r}_{\boldsymbol{ij}}^{2}\right)$$

$$V_{ij}^{kl}(x) = exp\left(-a_{kl}x_{\boldsymbol{ij}}^{2}\right)$$

$$\langle\psi'|V|\psi\rangle = \sum_{\hat{p}\in P_{A.S}} sign(\hat{p}) \sum_{k,l}\sum_{i<j} C_{kl}\left\langle st\middle|O_{ij}^{k}\middle|\hat{p}st\right\rangle \prod_{a=x,y,z}\left\langle {\psi'}^{a}\middle|V_{ij}^{kl}(x)\middle|\hat{p}\psi^{a}\right\rangle$$