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

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

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

Where $\boldsymbol{x}^T = (x_1, x_2, \dots . x_N)$. for simplicity we'll drop the index x from $A, B, \boldsymbol{s}$.

Denote

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

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

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

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

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

Using the integrals in the appendix we get

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

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

==

Using the integrals in the appendix we get

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

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

==

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

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

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

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

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

==

APPENDIX

$$\int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dx_1 \dots dx_N \; exp\left(-\frac{1}{2} \boldsymbol{x}^T A \boldsymbol{x} + \boldsymbol{b} \cdot \boldsymbol{x} \right) = \sqrt{\frac{(2\pi)^N}{\det A}} \, exp\left(\frac{1}{2} \boldsymbol{b}^T A^{-1} \boldsymbol{b} \right)$$

$$\int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dx_1 \dots dx_N \; x_i^n exp\left(-\frac{1}{2} \boldsymbol{x}^T A \boldsymbol{x} + \boldsymbol{b} \cdot \boldsymbol{x} \right)$$

$$= \frac{\partial^n}{\partial b_i^n} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dx_1 \dots dx_N \; exp\left(-\frac{1}{2} \boldsymbol{x}^T A \boldsymbol{x} + \boldsymbol{b} \cdot \boldsymbol{x} \right)$$

$$\int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dx_1 \dots dx_N \; x_i exp\left(-\frac{1}{2} \boldsymbol{x}^T A \boldsymbol{x} + \boldsymbol{b} \cdot \boldsymbol{x} \right) = \frac{\partial}{\partial b_i} \sqrt{\frac{(2\pi)^N}{\det A}} \, exp\left(\frac{1}{2} \boldsymbol{b}^T A^{-1} \boldsymbol{b} \right)$$

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

$$\int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dx_1 \dots dx_N \; x_i^2 exp\left(-\frac{1}{2} \boldsymbol{x}^T A \boldsymbol{x} + \boldsymbol{b} \cdot \boldsymbol{x} \right) = \frac{\partial^2}{\partial b_i^2} \sqrt{\frac{(2\pi)^N}{\det A}} \, exp\left(\frac{1}{2} \boldsymbol{b}^T A^{-1} \boldsymbol{b} \right)$$

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

The energy matrix element are

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

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

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

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

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

$$\left(\left((\mathbb{A}^{\boldsymbol{x}})^{-\mathbf{1}} (B_1^x \boldsymbol{s}_1^x + B_2^x \boldsymbol{s}_2^x) \right)_i^2 + \left((\mathbb{A}^{\boldsymbol{x}})^{-\mathbf{1}} \right)_{\boldsymbol{ii}} \right)$$

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

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

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

The basis function are $\psi_{3D} = \prod_{a=x,y,z} \psi^a_{pbc}$ Using basis with periodic boundary conditions,

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

$$\psi^a_{pbc} = \sum_{\boldsymbol{b}^a=-\infty}^{\infty} \psi^a(A^a, B^a, \boldsymbol{s}^a, \boldsymbol{x}^a - L\boldsymbol{b}^a)$$

Where $\boldsymbol{x}^a = (x^a_1 \dots x^a_N)$ and $\boldsymbol{b}^a = (b^a_1 \dots b^a_N)$ and the sum is all over $b^a_i = \dots - 2, -1, 0, 1, 2 \dots$

The kinetic energy is

$$T = \sum_{a=1}^{3} \sum_{i=1}^{N} \frac{1}{2m_i} \frac{\partial^2}{\partial \left(x^a_i\right)^2}$$

$$\langle \psi'_{3D} | T | \psi_{3D} \rangle = \sum_{a=1}^{3} \langle \psi'^z | \langle \psi'^y | \left\langle \psi'^x \middle| \sum_{i=1}^{N} \frac{1}{2m_i} \frac{\partial^2}{\partial \left(x^a_i\right)^2} \middle| \psi^x \right\rangle | \psi^y \rangle | \psi^z \rangle$$

$$\left\langle \psi'^a \middle| \sum_{i=1}^{N} \frac{1}{2m_i} \frac{\partial^2}{\partial \left(x^a_i\right)^2} \middle| \psi^a \right\rangle = \sum_{i=1}^{N} \frac{-\hbar^2}{2m_i} \left\langle \psi'^a \middle| \frac{\partial^2}{\partial \left(x^a_i\right)^2} \middle| \psi^a \right\rangle$$

$$\left\langle \psi'^a \middle| \frac{\partial^2}{\partial \left(x^a_i\right)^2} \middle| \psi^a \right\rangle = \int_0^L \dots \int_0^L dx^a_1 \dots dx^a_N \, \psi'^a \frac{\partial^2}{\partial \left(x^a_i\right)^2} \, \psi^a$$

$$\int_0^L dx^a_i \psi'^a \frac{\partial^2}{\partial \left(x^a_i\right)^2} \, \psi^a = -\int_0^L dx^a_i \frac{\partial}{\partial \left(x^a_i\right)} \psi'^a \frac{\partial}{\partial \left(x^a_i\right)} \, \psi^a$$

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

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

$$\frac{\partial}{\partial\left(x_i^a\right)}\left(-\frac{1}{2}(\boldsymbol{x}^a)^T A^a(\boldsymbol{x}^a)-\frac{1}{2}(\boldsymbol{x}^a-\boldsymbol{s}^a)^T B^a(\boldsymbol{x}^a-\boldsymbol{s}^a)\right)$$

$$=-\frac{1}{2}\frac{\partial}{\partial\left(x_i^a\right)}\sum_{kl}^{N} A_{kl}^a x_k^a x_l^a + B_{kl}^a(x_k^a-s_k^a)(x_l^a-s_l^a)$$

$$=-\frac{1}{2}\sum_{kl}^{N} A_{kl}^a\delta_{ki}x_l^a + A_{kl}^a x_k^a\delta_{li} + B_{kl}^a\delta_{ki}(x_l^a-s_l^a) + B_{kl}^a(x_k^a-s_k^a)\delta_{li}$$

$$=-\frac{1}{2}\sum_{l}^{N} A_{il}^a x_l^a - \frac{1}{2}\sum_{k}^{N} A_{ki}^a x_k^a - \frac{1}{2}\sum_{l}^{N} B_{il}^a(x_l^a-s_l^a) - \frac{1}{2}\sum_{k}^{N} B_{ki}^a(x_k^a-s_k^a)$$

$$=-\sum_{k}^{N} A_{ik}^a x_k^a + B_{ik}^a(x_k^a-s_k^a)$$

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

$$-\int_0^L dx_i^a\,\frac{\partial}{\partial\left(x_i^a\right)}\psi'^a\,\frac{\partial}{\partial\left(x_i^a\right)}\,\psi^a$$

$$=-\int_0^L dx_i^a[A^a\boldsymbol{x}^a + B^a(\boldsymbol{x}^a-\boldsymbol{s}^a)]_i[A'^a\boldsymbol{x}^a + B'^a(\boldsymbol{x}^a-\boldsymbol{s}'^a)]_i\psi'^a\,\psi^a$$

$$\frac{\partial^2\psi^a}{\partial\left(x_i^a\right)^2} = -\frac{\partial}{\partial\left(x_i^a\right)}\left(\psi^a\sum_{k}^{N} A_{ik}^a x_k^a + B_{ik}^a(x_k^a-s_k^a)\right)$$

$$=-\frac{\partial}{\partial\left(x_i^a\right)}\psi^a\sum_{k}^{N} A_{ik}^a x_k^a + B_{ik}^a(x_k^a-s_k^a) + \psi^a\frac{\partial}{\partial\left(x_i^a\right)}\sum_{k}^{N} A_{ik}^a x_k^a + B_{ik}^a(x_k^a-s_k^a)$$

$$=\psi^a\sum_{k}^{N} A_{ik}^a x_k^a + B_{ik}^a(x_k^a-s_k^a)\sum_{k}^{N} A_{ik}^a x_k^a + B_{ik}^a(x_k^a-s_k^a) + \psi^a(A_{ii}^a + B_{ii}^a)$$

$$=\psi^a\left(\left(A^a\boldsymbol{x}^{\boldsymbol{a}} + B^a(\boldsymbol{x}^{\boldsymbol{a}}-\boldsymbol{s}^{\boldsymbol{a}})\right)_i^2 + (A_{ii}^a + B_{ii}^a)\right)$$

$$\sum_{i=1}^{N}\frac{-\hbar^2}{2m_i}\left\langle\psi'^a\middle|\frac{\partial^2}{\partial\left(x_i^a\right)^2}\middle|\psi^a\right\rangle =$$

$$\sum_{i=1}^{N}\frac{-\hbar^2}{2m_i}\left\langle\psi'^a\middle|\left(A^a\boldsymbol{x^a}+B^a(\boldsymbol{x^a}-\boldsymbol{s^a})\right)_i^2+(A_{ii}^a+B_{ii}^a)\middle|\psi^a\right\rangle$$

$$\sum_{i=1}^{N}\frac{-\hbar^2}{2m_i}\left\langle\psi'^a\middle|\left(A^a\boldsymbol{x^a}+B^a(\boldsymbol{x^a}-\boldsymbol{s^a})\right)_i^2\middle|\psi^a\right\rangle+\sum_{i=1}^{N}\frac{-\hbar^2}{2m_i}(A_{ii}^a+B_{ii}^a)\langle\psi'^a|\psi^a\rangle$$

$$\sum_{i=1}^{N}\frac{-\hbar^2}{2m_i}(A_{ii}^a+B_{ii}^a)\langle\psi'^a|\psi^a\rangle=\frac{-\hbar^2}{2}\langle\psi'^a|\psi^a\rangle Tr\left((A^a+B^a)\Lambda\right)$$

$$\Lambda_{\mathrm{jj}}=\frac{1}{m_j}$$

$$=\sum_{i=1}^{N}\frac{-\hbar^2}{2m_i}\int_0^L\dots\int_0^L dx_1^a\dots dx_N^a\ \psi^a\left(\left(A^a\boldsymbol{x^a}+B^a(\boldsymbol{x^a}-\boldsymbol{s^a})\right)_i^2\right)\psi^a$$

There are N integrals.

Define a new $\boldsymbol{x}^a$ as $\boldsymbol{x}^a=\boldsymbol{x}^a-L\boldsymbol{b}'^a$ and replace $\boldsymbol{b}^a-\boldsymbol{b}'^a$ by $\Delta\boldsymbol{b}^a$ and make the sum over $\Delta\boldsymbol{b}^a$ instead of $\boldsymbol{b}^a$.

$$\sum_{\boldsymbol{b}'^a}\sum_{\Delta\boldsymbol{b}^a}\int_{-Lb_1'^a}^{L-Lb_1'^a}\dots\int_{-Lb_N'^a}^{L-Lb_N'^a}dx_1^a\dots dx_N^a$$

$$\times\,exp\left(-\frac{1}{2}(\boldsymbol{x}^a)^TA'^a(\boldsymbol{x}^a)-\frac{1}{2}(\boldsymbol{x}^a-\boldsymbol{s}'^a)^TB'^a(\boldsymbol{x}^a-\boldsymbol{s}'^a)\right)$$

$$\times\,exp\left(-\frac{1}{2}(\boldsymbol{x}^a-L\Delta\boldsymbol{b}^a)^TA^a(\boldsymbol{x}^a-L\Delta\boldsymbol{b}^a)-\frac{1}{2}(\boldsymbol{x}^a-L\Delta\boldsymbol{b}^a-\boldsymbol{s}^a)^TB^a(\boldsymbol{x}^a-L\Delta\boldsymbol{b}^a-\boldsymbol{s}^a)\right)$$

$$=\int_0^L\dots\int_0^L dx_1^a\dots dx_N^a\ \psi^a(A'^a,B'^a,\boldsymbol{s}'^a,\boldsymbol{x}^a)\,V_{ijk}^{pbc,a}\left(x_{ij}^a\right)\psi^a(A^a,B^a,\boldsymbol{s}^a,\boldsymbol{x}^a)$$

There are N integrals.

Write the potential as

$$V_{ij}^a\left(x_{ij}^a\right)=\int dyV^a(y)\delta\left(y-x_{ij}^a\right)$$

And first we calculate the integral

$$\int_0^L \ldots \int_0^L dx_1^a \ldots dx_N^a \, \psi'^a \sum_{q^a} \delta\left(y - x_{ij}^a + Lq^a\right) \psi^a$$

Where $x_{ij}^a = x_i^a - x_j^a$ but in the most general case

$$x_{ij}^a = \sum_{m=1}^N C_m^{ij} x_m^a$$

Or $$x_{ij}^a = \boldsymbol{C}^{ij} \cdot \boldsymbol{x^a}$$

So the integral is

$$\sum_{\boldsymbol{b}'^a} \sum_{\boldsymbol{b}^a} \int_0^L \ldots \int_0^L dx_1^a \ldots dx_N^a$$

$$\times\, exp\left(-\frac{1}{2}(\boldsymbol{x}^a - L\boldsymbol{b}'^a)^T A'^a (\boldsymbol{x}^a - L\boldsymbol{b}'^a) - \frac{1}{2}(\boldsymbol{x}^a - L\boldsymbol{b}'^a - \boldsymbol{s}'^a)^T B'^a (\boldsymbol{x}^a - L\boldsymbol{b}'^a - \boldsymbol{s}'^a)\right)$$

$$\times\, exp\left(-\frac{1}{2}(\boldsymbol{x}^a - L\boldsymbol{b}^a)^T A^a (\boldsymbol{x}^a - L\boldsymbol{b}^a) - \frac{1}{2}(\boldsymbol{x}^a - L\boldsymbol{b}^a - \boldsymbol{s}^a)^T B^a (\boldsymbol{x}^a - L\boldsymbol{b}^a - \boldsymbol{s}^a)\right)$$

$$\times \sum_{q^a=-\infty}^{\infty} \delta\left(y - \boldsymbol{C}^{ij} \cdot \boldsymbol{x^a} + Lq^a\right)$$

Define a new $\boldsymbol{x}^a$ as $\boldsymbol{x}^a = \boldsymbol{x}^a - L\boldsymbol{b}'^a$ and replace $\boldsymbol{b}^a - \boldsymbol{b}'^a$ by $\Delta\boldsymbol{b}^a$ and make the sum over $\Delta\boldsymbol{b}^a$ instead of $\boldsymbol{b}^a$.

$$\sum_{\boldsymbol{b}'^a} \sum_{\Delta\boldsymbol{b}^a} \int_{-Lb_1'^a}^{L-Lb_1'^a} \ldots \int_{-Lb_N'^a}^{L-Lb_N'^a} dx_1^a \ldots dx_N^a$$

$$\times\, exp\left(-\frac{1}{2}(\boldsymbol{x}^a)^T A'^a (\boldsymbol{x}^a) - \frac{1}{2}(\boldsymbol{x}^a - \boldsymbol{s}'^a)^T B'^a (\boldsymbol{x}^a - \boldsymbol{s}'^a)\right)$$

$$\times\, exp\left(-\frac{1}{2}(\boldsymbol{x}^a - L\Delta\boldsymbol{b}^a)^T A^a (\boldsymbol{x}^a - L\Delta\boldsymbol{b}^a) - \frac{1}{2}(\boldsymbol{x}^a - L\Delta\boldsymbol{b}^a - \boldsymbol{s}^a)^T B^a (\boldsymbol{x}^a - L\Delta\boldsymbol{b}^a - \boldsymbol{s}^a)\right)$$

$$\times \sum_{q^a=-\infty}^{\infty} \delta\left(y - \boldsymbol{C}^{ij} \cdot (\boldsymbol{x^a} + L\boldsymbol{b}'^a) + Lq^a\right)$$

Now define a new q^a as $q^a = q^a - \boldsymbol{C}^{ij} \cdot \boldsymbol{b}'^a$ the result of the sum over the old and the new q^a is identical because $\boldsymbol{b}'^a$ is fixed.

$$
= \sum_{\boldsymbol{b}'^a} \sum_{\Delta \boldsymbol{b}^a} \int_{-Lb_1'^a}^{L-Lb_1'^a} \dots \int_{-Lb_N'^a}^{L-Lb_N'^a} dx_1^a \dots dx_N^a
$$

$$
\times\, exp\left(-\frac{1}{2}(\boldsymbol{x}^a)^T A'^a(\boldsymbol{x}^a) - \frac{1}{2}(\boldsymbol{x}^a - \boldsymbol{s}'^a)^T B'^a(\boldsymbol{x}^a - \boldsymbol{s}'^a)\right)
$$

$$
\times\, exp\left(-\frac{1}{2}(\boldsymbol{x}^a - L\Delta\boldsymbol{b}^a)^T A^a(\boldsymbol{x}^a - L\Delta\boldsymbol{b}^a) - \frac{1}{2}(\boldsymbol{x}^a - L\Delta\boldsymbol{b}^a - \boldsymbol{s}^a)^T B^a(\boldsymbol{x}^a - L\Delta\boldsymbol{b}^a - \boldsymbol{s}^a)\right)
$$

$$
\sum_{q^a=-\infty}^{\infty} \delta\left(y - \boldsymbol{C}^{ij} \cdot \boldsymbol{x}^{\boldsymbol{a}} + Lq^a\right)
$$

Now the integrand is independent of $\boldsymbol{b}'^a$ and the sum over $\boldsymbol{b}'^a$ change the integration limit to $[-\infty, \infty]$. Renaming $\Delta\boldsymbol{b}^a$ as $\boldsymbol{b}^a$ we find

$$
= \sum_{q^a} \sum_{\boldsymbol{b}^a} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} dx_1^a \dots dx_N^a\, \delta\left(y - \boldsymbol{C}^{ij} \cdot \boldsymbol{x}^{\boldsymbol{a}} + Lq^a\right)
$$

$$
\times\, exp\left(-\frac{1}{2}(\boldsymbol{x}^a)^T A'^a(\boldsymbol{x}^a) - \frac{1}{2}(\boldsymbol{x}^a - \boldsymbol{s}'^a)^T B'^a(\boldsymbol{x}^a - \boldsymbol{s}'^a)\right)
$$

$$
\times\, exp\left(-\frac{1}{2}(\boldsymbol{x}^a - L\boldsymbol{b}^a)^T A^a(\boldsymbol{x}^a - L\boldsymbol{b}^a) - \frac{1}{2}(\boldsymbol{x}^a - L\boldsymbol{b}^a - \boldsymbol{s}^a)^T B^a(\boldsymbol{x}^a - L\boldsymbol{b}^a - \boldsymbol{s}^a)\right)
$$

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

Using

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

We get

$$
= \sum_{q^a} \sum_{\boldsymbol{b}^a} \int \frac{dk}{2\pi} \exp\left(ik(y + Lq^a)\right) \int d\boldsymbol{x}^a\ exp\left(-ik\boldsymbol{C}^{ij} \cdot \boldsymbol{x}^a\right)
$$

$$
\times\, exp\left(-\frac{1}{2}(\boldsymbol{x}^a)^T A'^a(\boldsymbol{x}^a) - \frac{1}{2}(\boldsymbol{x}^a - \boldsymbol{s}'^a)^T B'^a(\boldsymbol{x}^a - \boldsymbol{s}'^a)\right)
$$

$$
\times\, exp\left(-\frac{1}{2}(\boldsymbol{x}^a - L\boldsymbol{b}^a)^T A^a(\boldsymbol{x}^a - L\boldsymbol{b}^a) - \frac{1}{2}(\boldsymbol{x}^a - L\boldsymbol{b}^a - \boldsymbol{s}^a)^T B^a(\boldsymbol{x}^a - L\boldsymbol{b}^a - \boldsymbol{s}^a)\right)
$$

$$(\boldsymbol{x}^a - L\boldsymbol{b}^a)^T A(\boldsymbol{x}^a - L\boldsymbol{b}^a) = (\boldsymbol{x}^a)^T A(\boldsymbol{x}^a) - L(\boldsymbol{x}^a)^T A(\boldsymbol{b}^a) - L(\boldsymbol{b}^a)^T A(\boldsymbol{x}^a) + L^2(\boldsymbol{b}^a)^T A(\boldsymbol{b}^a)$$

A and B are symmetric matrix so $(\boldsymbol{x}^a)^T A(\boldsymbol{b}^a) + (\boldsymbol{b}^a)^T A(\boldsymbol{x}^a) = 2(A\boldsymbol{b}^a)\cdot\boldsymbol{x}^a$

$$= \sum_{q^a}\sum_{\boldsymbol{b}^a} exp\left(-\frac{L^2}{2}(\boldsymbol{b}^a)^T(A^a + B^a)(\boldsymbol{b}^a) - LB^a\boldsymbol{b}^a\cdot\boldsymbol{s}^a\right)$$

$$\int\frac{dk}{2\pi}exp\big(ik(y + Lq^a)\big)$$

$$\int d\boldsymbol{x}^a\ exp\left(-\frac{1}{2}(\boldsymbol{x}^a)^T(A'^a + A^a)(\boldsymbol{x}^a) - \big(ik\boldsymbol{C}^{ij} - L(A^a + B^a)\boldsymbol{b}^a\big)\cdot\boldsymbol{x}^a\right)$$

$$exp\left(-\frac{1}{2}(\boldsymbol{x}^a - \boldsymbol{s}'^a)^T B'^a(\boldsymbol{x}^a - \boldsymbol{s}'^a) - \frac{1}{2}(\boldsymbol{x}^a - \boldsymbol{s}^a)^T B^a(\boldsymbol{x}^a - \boldsymbol{s}^a)\right)$$

Substitute

$$-\frac{1}{2}(\boldsymbol{x}^a - \boldsymbol{s}'^a)^T B'^a(\boldsymbol{x}^a - \boldsymbol{s}'^a) - \frac{1}{2}(\boldsymbol{x}^a - \boldsymbol{s}^a)^T B^a(\boldsymbol{x}^a - \boldsymbol{s}^a)$$

$$= -\frac{1}{2}(\boldsymbol{x}^a)^T(B^a + B'^a)(\boldsymbol{x}^a) + (B^a\boldsymbol{s}^a + B'^a\boldsymbol{s}'^a)\cdot\boldsymbol{x}^a - \frac{1}{2}(\boldsymbol{s}^a)^T B^a(\boldsymbol{s}^a) - \frac{1}{2}(\boldsymbol{s}'^a)^T B'^a(\boldsymbol{s}'^a)$$

To get

$$= \sum_{q^a}\sum_{\boldsymbol{b}^a} exp\left(-\frac{1}{2}(L\boldsymbol{b}^a)^T A^a(L\boldsymbol{b}^a) - \frac{1}{2}(L\boldsymbol{b}^a + \boldsymbol{s}^a)^T B^a(L\boldsymbol{b}^a + \boldsymbol{s}^a) - \frac{1}{2}(\boldsymbol{s}'^a)^T B'^a(\boldsymbol{s}'^a)\right)$$

$$\int\frac{dk}{2\pi}exp\big(ik(y + Lq^a)\big)$$

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

$$\times\, exp\Big(\big(-ik\boldsymbol{C}^{ij} + L(A^a + B^a)\boldsymbol{b}^a + B^a\boldsymbol{s}^a + B'^a\boldsymbol{s}'^a\big)\cdot\boldsymbol{x}^a\Big)$$

For the last integral we use the formula

(1) $$\int d\boldsymbol{x}e^{-\frac{1}{2}\boldsymbol{xAx}}\,e^{b\cdot x} = \sqrt{\frac{(2\pi)^N}{\det\boldsymbol{A}}}\,e^{\frac{1}{2}\boldsymbol{bA^{-1}b}}$$

$$= \sqrt{\frac{(2\pi)^N}{det\,\mathbb{A}^a}}$$

$$\times \sum_{q^a} \sum_{\boldsymbol{b}^a} exp\left(-\frac{1}{2}(L\boldsymbol{b}^a)^T A^a (L\boldsymbol{b}^a) - \frac{1}{2}(L\boldsymbol{b}^a + \boldsymbol{s}^a)^T B^a (L\boldsymbol{b}^a + \boldsymbol{s}^a) - \frac{1}{2}(\boldsymbol{s}'^a)^T B'^a (\boldsymbol{s}'^a)\right)$$

$$\int \frac{dk}{2\pi} exp\big(ik(y + Lq^a)\big)$$

$$\times\, exp\left(\frac{1}{2}\left(-ik\boldsymbol{C}^{ij} + \boldsymbol{d}^a\right)^T \mathbb{A}^{a^{-1}} \left(-ik\boldsymbol{C}^{ij} + \boldsymbol{d}^a\right)\right)$$

Where

$$\boldsymbol{d}^a = L(A^a + B^a)\boldsymbol{b}^a + B^a\boldsymbol{s}^a + B'^a\boldsymbol{s}'^a$$

$$\mathbb{A}^a = A'^a + A^a + B'^a + B^a$$

Rewrite the exponent in the last integral,

$$\left(-ik\boldsymbol{C}^{ij} + \boldsymbol{d}^a\right)^T \mathbb{A}^{a^{-1}} \left(-ik\boldsymbol{C}^{ij} + \boldsymbol{d}^a\right)$$

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

$$-(\boldsymbol{d}^a)^T \mathbb{A}^{a^{-1}} \left(ik\boldsymbol{C}^{ij}\right)$$

$$-\left(ik\boldsymbol{C}^{ij}\right)^T \mathbb{A}^{a^{-1}} (\boldsymbol{d}^a)$$

$$+(\boldsymbol{d}^a)^T \mathbb{A}^{a^{-1}} (\boldsymbol{d}^a)$$

To get the matrix element of two delta function

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

$$\times\, exp\left(-\frac{1}{2}(L\boldsymbol{b}^a)^T A^a (L\boldsymbol{b}^a) - \frac{1}{2}(L\boldsymbol{b}^a + \boldsymbol{s}^a)^T B^a (L\boldsymbol{b}^a + \boldsymbol{s}^a) - \frac{1}{2}(\boldsymbol{s}'^a)^T B'^a (\boldsymbol{s}'^a)\right)$$

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

For the last integral using again the formula

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

$$= \frac{1}{\sqrt{(\boldsymbol{C}^{ij})^T \mathbb{A}^{a^{-1}} (\boldsymbol{C}^{ij})}} \frac{1}{\sqrt{2\pi}} \sqrt{\frac{(2\pi)^N}{det\, \mathbb{A}^a}} \sum_{q^a} \sum_{\boldsymbol{b}^a} exp\left(\frac{1}{2}(\boldsymbol{d}^a)^T \mathbb{A}^{a^{-1}} (\boldsymbol{d}^a)\right)$$

$$\times\, exp\left(-\frac{1}{2}(L\boldsymbol{b}^a)^T A^a (L\boldsymbol{b}^a) - \frac{1}{2}(L\boldsymbol{b}^a + \boldsymbol{s}^a)^T B^a (L\boldsymbol{b}^a + \boldsymbol{s}^a) - \frac{1}{2}(\boldsymbol{s}'^a)^T B'^a (\boldsymbol{s}'^a)\right)$$

$$exp\left(-\frac{\left(y + Lq^a - \left(\mathbb{A}^{a^{-1}}\boldsymbol{d}^a\right)\cdot \boldsymbol{C}^{ij}\right)^{\boldsymbol{2}}}{2(\boldsymbol{C}^{ij})^T\mathbb{A}^{a^{-1}}(\boldsymbol{C}^{ij})}\right)$$

Denote $r = -Lq^a + \left(\mathbb{A}^{a^{-1}}\boldsymbol{d}^a\right)\cdot \boldsymbol{C}^{ij}$ and $s = \left(\boldsymbol{C}^{ij}\right)^T \mathbb{A}^{a^{-1}}\left(\boldsymbol{C}^{ij}\right)$

The y dependent part is

$$exp\left(-\frac{(y-r)^{\boldsymbol{2}}}{2s}\right)$$

To calculate the matrix element of the potential $\left\langle \psi'^a \middle| V_{ijk}^{pbc,a} \middle| \psi^a \right\rangle$ *we need took integral over* $dy_1 dy_2$ *of the last expression*

$$\left\langle \psi'^a \middle| V_{ijk}^{pbc,a} \middle| \psi^a \right\rangle = \int dy e^{-\frac{\Lambda^2}{4}y^2} \langle \psi'^a | \textstyle\sum_{q^a} \delta\left(y - x_{ij}^a - Lq^a\right)\delta\, |\psi^a\rangle$$

And the integral over $\boldsymbol{y}$ is

$$\int dy\, exp\left(-\frac{\Lambda^2}{4}y^2 - \frac{(y-r)^{\boldsymbol{2}}}{2s}\right)$$

$$= exp\left(-\frac{r^{\boldsymbol{2}}}{2s}\right)\int dy\, exp\left(-\frac{1}{2}\left(\frac{\Lambda^2}{2} + \frac{1}{s}\right)y^2 + \frac{r}{s}y\right)$$

$$= \sqrt{\frac{2\pi}{\frac{\Lambda^2}{2} + \frac{1}{s}}}\, exp\left(-\frac{\Lambda^2}{4}\left(\frac{1}{\frac{\Lambda^2 s}{2} + 1}\right)r^2\right)$$

Finally

$$\left\langle \psi'^a \middle| V_{ij}^{pbc,a} \middle| \psi^a \right\rangle = \sqrt{\frac{(2\pi)^N}{det\, \mathbb{A}^a}} \sum_{q^a}\sum_{\boldsymbol{b}^a} exp\left(\frac{1}{2}(\boldsymbol{d}^a)^T \mathbb{A}^{a^{-1}} (\boldsymbol{d}^a)\right)$$

$$\times\, exp\left(-\frac{1}{2}(L\boldsymbol{b}^a)^T A^a (L\boldsymbol{b}^a) - \frac{1}{2}(L\boldsymbol{b}^a + \boldsymbol{s}^a)^T B^a (L\boldsymbol{b}^a + \boldsymbol{s}^a) - \frac{1}{2}(\boldsymbol{s}'^a)^T B'^a (\boldsymbol{s}'^a)\right)$$

$$\sqrt{\frac{1}{\frac{\Lambda^2 s}{2}+1}}\, exp\left(-\frac{\Lambda^2}{4}\left(\frac{1}{\frac{\Lambda^2 s}{2}+1}\right) r^2\right)$$

$$r = -Lq^a + \left(\mathbb{A}^{a^{-1}} \boldsymbol{d}^a\right)\cdot \boldsymbol{C}^{ij}$$

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

$$\boldsymbol{d}^a = L(A^a + B^a)\boldsymbol{b}^a + B^a \boldsymbol{s}^a + B'^a \boldsymbol{s}'^a$$

$$\mathbb{A}^a = A'^a + A^a + B'^a + B^a$$

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

$$\times \sum_{\boldsymbol{b}^a} exp\left(-\frac{1}{2}(L\boldsymbol{b}^a)^T A^a (L\boldsymbol{b}^a) - \frac{1}{2}(L\boldsymbol{b}^a + \boldsymbol{s}^a)^T B^a (L\boldsymbol{b}^a + \boldsymbol{s}^a) - \frac{1}{2}(\boldsymbol{s}'^a)^T B'^a (\boldsymbol{s}'^a)\right)$$

$$\times\, exp\left(\frac{1}{2}(\boldsymbol{d}^a)^T \mathbb{A}^{a^{-1}} (\boldsymbol{d}^a)\right)$$

Denote

$$\langle \psi'^a | \psi^a \rangle = \sqrt{\frac{(2\pi)^N}{det\, \mathbb{A}^a}}\, exp\left(\frac{1}{2}(\boldsymbol{d}^a)^T \mathbb{A}^{a^{-1}} (\boldsymbol{d}^a)\right)$$

$$\times\, exp\left(-\frac{1}{2}(L\boldsymbol{b}^a)^T A^a (L\boldsymbol{b}^a) - \frac{1}{2}(L\boldsymbol{b}^a + \boldsymbol{s}^a)^T B^a (L\boldsymbol{b}^a + \boldsymbol{s}^a) - \frac{1}{2}(\boldsymbol{s}'^a)^T B'^a (\boldsymbol{s}'^a)\right)$$

And

$$\langle \psi'^a | \psi^a \rangle_{pbc} = \sum_{\boldsymbol{b}^a} \langle \psi'^a | \psi^a \rangle$$

$$\left\langle \psi'^a \middle| V_{ij}^{pbc,a} \middle| \psi^a \right\rangle = \sum_{q^a} \sum_{\boldsymbol{b}^a} \langle \psi'^a | \psi^a \rangle \sqrt{\frac{1}{\frac{\Lambda^2 s}{2}+1}}\, exp\left(-\frac{\Lambda^2}{4}\left(\frac{1}{\frac{\Lambda^2 s}{2}+1}\right) r^2\right)$$

$$\left\langle \psi'^a \middle| V_{ij}^{pbc,a} \middle| \psi^a \right\rangle = \sum_{q^a} \sum_{\boldsymbol{b}^a} \langle \psi'^a | \psi^a \rangle \sqrt{\frac{1}{\frac{\Lambda^2 s}{2}+1}}\, exp\left(-\frac{\Lambda^2}{4}\left(\frac{1}{\frac{\Lambda^2 s}{2}+1}\right) r^2\right)$$

$$r = Lq^{a} + \left(\mathbb{A}^{a-1}\boldsymbol{d}^{a}\right) \cdot \boldsymbol{C}^{ij}$$

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