**gaussian\_int((nxa-i+nxb-j), gamma)**

**double gaussian\_overlap\_ref(int nxa, double alp\_a, double Xa, int nxb, double alp\_b, double Xb )** computes

Consider that Gaussians are given as:

Then:

The basic overlap is:

Because:

Where:

Because:

Because:

Now consider:

Thus, without normalization:

This is done by the function:

**double gaussian\_moment\_ref(int nx, double alp, double X, int nxa,double alp\_a, double Xa, int nxb,double alp\_b, double Xb)** computes

Using the Gaussian contraction formula:

Where:

Then express the middle GTO in terms of the center of the contraction of GTOs and :

So:

Then:

**Now compute the derivatives:**

- directly

,

.