$$g_{nl}(\vec{r},\alpha,\vec{A}) = N_{nl}(\alpha)\,\|\vec{r}-\vec{A}\|^{n-l-1}(x-A_x)^{l_x}(y-A_y)^{l_y}(z-A_z)^{l_z}\,e^{-\alpha\|\vec{r}-\vec{A}\|^2}$$

$n \equiv l+1$ $\quad l = l_x+l_y+l_z \quad i\equiv l_x \quad j\equiv l_y \quad k\equiv l_z$

↓ Normierung wird vernachlässigt, da sie im Programm auch zu späterer Stelle erfolgt

$\Rightarrow N_{nl}(\alpha)\equiv 1$

$$g_{ijk}(\vec{r};\alpha,\vec{A}) = (x-A_x)^i(y-A_x)^j(z-A_z)^k\,e^{-\alpha\|\vec{r}-\vec{A}\|^2}$$

↓

$$g_i(r_p;\alpha,A_p) = (r_p-A_p)^i\,e^{-\alpha(r_p-A_p)^2}$$

$$S_{ijk,lmn}^{A,B} = \int g_{ijk}(\vec{r};\alpha,\vec{A})\,g_{lmn}(\vec{r};\beta,\vec{B})\,d^3r$$

$$= \int (x-A_x)^i(x-B_x)^l\,e^{-\alpha(x-A_x)^2-\beta(x-B_x)^2}\,dx \;\Big\}\; S_{il}^{A_x,B_x}$$

$$+ \int (y-A_y)^j(y-B_y)^m\,e^{-\alpha(y-A_y)^2-\beta(y-B_y)^2}\,dy \;\Big\}\; S_{jm}^{A_y,B_y}$$

$$+ \int (z-A_z)^k(z-B_z)^n\,e^{-\alpha(z-A_z)^2-\beta(z-B_z)^2}\,dz \;\Big\}\; S_{kn}^{A_z,B_z}$$

$$T_{il}^{A_p B_p} = -\frac{1}{2}\int g_i(r_p;\alpha,A_p)\,\frac{\partial^2}{\partial r_p^2}\,g_l(r_p;\beta,B_p)\,dr_p =$$

$$= -\frac{1}{2}\int (r_p-A_p)^i\,e^{-\alpha(r_p-A_p)^2}\,\frac{\partial^2}{\partial r_p^2}\,(r_p-B_p)^l\,e^{-\beta(r_p-B_p)^2}$$

$$= -\frac{1}{2}\int (r_p-A_p)^i\,e^{-\alpha(r_p-A_p)^2}\,\frac{\partial}{\partial r_p}\Big[l\cdot(r_p-B_p)^{l-1}e^{-\beta(r_p-B_p)^2} + (r_p-B_p)^l\,e^{-\beta(r_p-B_p)^2}\cdot(-2\beta(r_p-B_p))\Big]$$

$$= -\frac{1}{2}\int (r_p-A_p)^i\,e^{-\alpha(r_p-A_p)^2}\Big[(l-1)\cdot l\cdot(r_p-B_p)^{l-2}e^{-\beta(r_p-B_p)^2} + l\cdot(r_p-B_p)^{l-1}e^{-\beta(r_p-B_p)^2}\cdot(-2\beta(r_p-B_p))$$

$$+ l\cdot(r_p-B_p)^{l-1}e^{-\beta(r_p-B_p)^2}\cdot(-2\beta(r_p-B_p)) + (r_p-B_p)^l\,e^{-\beta(r_p-B_p)^2}\cdot(-2\beta(r_p-B_p))^2$$

$$+ (-2\beta)(r_p-B_p)^l\,e^{-\beta(r_p-B_p)^2}\Big]$$

$$= -\frac{1}{2}\left[(\ell-1)\cdot\ell\cdot S_{i,\ell-2}^{A_p,B_p} - 2\beta\ell\cdot S_{i,\ell}^{A_p,B_p} - 2\beta\ell\cdot S_{i,\ell}^{A_p,B_p} + 4\beta^2 S_{i,\ell+2}^{A_p,B_p} - 2\beta S_{i,\ell}^{A_p,B_p}\right]$$

$$= -\frac{(\ell-1)\cdot\ell}{2} S_{i,\ell-2}^{A_p,B_p} - \frac{1}{2}(-4\beta\ell-2\beta) S_{i,\ell}^{A_p,B_p} - 2\beta^2 S_{i,\ell+2}^{A_p,B_p}$$

$$T_{i\ell}^{A_p,B_p} = -2\beta^2 S_{i,\ell+2}^{A_p,B_p} + \beta(2\ell+1) S_{i,\ell}^{A_p,B_p} - \frac{\ell(\ell-1)}{2}\cdot S_{i,\ell-2}^{A_p,B_p}$$