(Tip-４-２)　重なり積分・分子コア積分・交換積分の微分法整理

(ｉ) 関連基本諸量

$p = (\alpha+\beta)$　　$s = \alpha\beta/(\alpha+\beta)$

$q = (\gamma+\delta)$　　$t = \gamma\delta/(\gamma+\delta)$

$w = pq / (p+q)$

$x_p = (\alpha/p)\,x_a + (\beta/p)\,x_b$　　$y_p = (\alpha/p)\,y_a + (\beta/p)\,y_b$　　$z_p = (\alpha/p)\,z_a + (\beta/p)\,z_b$

$x_q = (\gamma/q)\,x_c + (\delta/q)\,x_d$　　(y, z について以下同様)

$\triangle x_a = x_p - x_a = (\alpha/p)\,x_a + (\beta/p)\,x_b - x_a = (\beta/p)(x_b - x_a) = (s/\alpha)(x_b - x_a)$

$\nabla x_p = x_p - x_s = (\alpha/p)\,x_a + (\beta/p)\,x_b - x_s$

$\nabla x_{pq} = x_p - x_q = \{(\alpha/p)\,x_a + (\beta/p)\,x_b\} - \{(\gamma/q)\,x_c + (\delta/q)\,x_d\}$

$R_{ab}{}^2 = (x_a - x_b)^2 + (y_a - y_b)^2 + (z_a - z_b)^2$

$R_{pq}{}^2 = (x_p - x_q)^2 + (y_p - y_q)^2 + (z_p - z_q)^2$

$R_s{}^2 = (x_p - x_s)^2 + (y_p - y_s)^2 + (z_p - z_s)^2$

(ⅱ) 基本式

(a) 重なり積分　(SaSb)　$= (\pi/p)^{3/2} \cdot \exp(-sR_{ab}{}^2)$

(b) コア積分１　＜SaSb＞　$= Z_s \cdot 2\pi/p \cdot \exp(-sR_{ab}{}^2)F0(p^{1/2}R_s)$

(c) コア積分２　[SaSb]　$= (\pi/p)^{3/2} \cdot s \cdot \exp(-sR_{ab}{}^2)\ (3 - 2sR_{ab}{}^2)$

(d) 交換積分　(SaSb｜ScSd) $= 2(\pi)^{5/2} \cdot (1/(pq(p+q)^{1/2})) \cdot \exp(-sR_{ab}{}^2)\exp(-tR_{cd}{}^2)F0((pq/(p+q))^{1/2}R_{pq})$

(ⅲ) 形式化

上記の式は、(a)から(c)では、F(Sa,Sb,Sc,Sd)= F(Sa,Sb)として、共通的に以下の如く形式化することができる。

$F(Sa,Sb,Sc,Sd) = K \cdot \exp Aab \cdot \exp Bcd \cdot F0(X)$

$\exp Aab = \exp(-sR_{ab}{}^2)$、　$\exp Bcd = 1$、　$F0=1$　　for (a)

$\exp Aab = \exp(-sR_{ab}{}^2)$、　$\exp Bcd = 1$、　$F0= F0(X)=F0(p^{1/2}R_s)$　　for (b)

$\exp Aab = \exp(-sR_{ab}{}^2)$、　$\exp Bcd = 1$、　$F0=(3-2sR_{ab}{}^2)$　　for (c)

$\exp Aab = \exp(-sR_{ab}{}^2)$、　$\exp Bcd = \exp(-tR_{cd}{}^2)$、$F0=F0(X)=F0((pq/(p+q))^{1/2}R_{pq})$　　for (d)

その他のＦは、以下の式から得られる。(但し、$x_a{}^0 = Sa$)

$F(x_a{}^n,x_b{}^m,x_c{}^k,x_d y_d) = 1/(2\alpha) \cdot \{\partial/\partial x_a\, F(x_a{}^{n-1},x_b{}^m,x_c{}^k,x_d y_d) + (n-1)\, F(x_a{}^{n-2},x_b{}^m,x_c{}^k,x_d y_d)\}$

$= 1/(2\beta) \cdot \{\partial/\partial x_b\, F(x_a{}^n,x_b{}^{m-1},x_c{}^k,x_d y_d) + (m-1)\, F(x_a{}^n,x_b{}^{m-2},x_c{}^k,x_d y_d)\}$

$= 1/(2\gamma) \cdot \{\partial/\partial x_c\, F(x_a{}^n,x_b{}^m,x_c{}^{k-1},x_d{}^l) + (k-1)\, F(x_a{}^n,x_b{}^m,x_c{}^{k-2},x_d y_d)\}$

$= 1/(2\delta) \cdot \{\partial/\partial y_d\, F(x_a{}^n,x_b{}^m,x_c{}^k,x_d)\}$

(ⅳ) 微分

(ⅳ-1) expAab の微分

$$1/(2\alpha)\cdot\partial/\partial x_a\ \mathrm{expAab} = 1/(2\alpha)\cdot\partial/\partial x_a \exp(-sR_{ab}^2) = 1/(2\alpha)\cdot\exp(-sR_{ab}^2)\cdot 2sR_{ab}\cdot(x_a-x_b)/R_{ab}$$
$$= \exp(-sR_{ab}^2)\cdot\triangle x_a$$

(ⅳ-2) ⊿の微分

$$1/(2\alpha)\cdot\partial/\partial x_a\ \triangle x_a = 1/(2\alpha)\cdot\partial/\partial x_a\,(x_p-x_a) = 1/(2\alpha)\cdot\partial/\partial x_a\,(\beta/p)\,(x_b-x_a) = -(\beta/\alpha)/(2p)$$
$$= 1/(2p)-1/(2\alpha)$$
$$1/(2\beta)\cdot\partial/\partial x_b\ \triangle x_a = 1/(2\alpha)\cdot\partial/\partial x_b\,(x_p-x_a) = 1/(2\alpha)\cdot\partial/\partial x_b\,(\beta/p)\,(x_b-x_a) = 1/(2p)$$
$$1/(2\beta)\cdot\partial/\partial x_b\ \triangle x_b = 1/(2\alpha)\cdot\partial/\partial x_a\,(x_p-x_b) = 1/(2\beta)\cdot\partial/\partial x_b\,(\alpha/p)\,(x_b-x_a) = 1/(2p)-1/(2\beta)$$

(ⅳ-3) ▽の微分

$$1/(2\alpha)\cdot\partial/\partial x_a\ \nabla x_p = 1/(2\alpha)\cdot\partial/\partial x_a\,(x_p-x_s) = 1/(2\alpha)\cdot(\alpha/p) = 1/(2p)$$
$$1/(2\alpha)\cdot\partial/\partial x_a\ \nabla x_{pq} = 1/(2\alpha)\cdot\partial/\partial x_a\,(x_p-x_q) = 1/(2\alpha)\cdot\{\alpha/p\} = 1/(2p)$$
$$1/(2\gamma)\cdot\partial/\partial x_c\ \nabla x_{pq} = 1/(2\gamma)\cdot\partial/\partial x_c\,(x_p-x_q) = 1/(2\gamma)\cdot\{-\gamma/q\} = -1/(2q)$$

(ⅳ-4) F0 の微分

$$1/(2\alpha)\cdot\partial/\partial x_a\,F0(X) = 1/(2\alpha)\cdot\partial F0(X)/\partial X\cdot\partial X/\partial x_a$$
$$= \begin{cases} 0 & \text{for (a)} \\ 2\triangle x_a & \text{for (c)} \\ (\exp(-X2)-F0(X))/X\cdot 1/(2\alpha)\cdot\partial X/\partial x_a \equiv \mathbf{FOX}\cdot 1/(2\alpha)\cdot\partial X/\partial x_a & \text{for (b) (d)} \end{cases}$$

ここに、(b)(d)に対する$\partial X/\partial x_a$の微分は

$$1/(2\alpha)\cdot\partial X/\partial x_a = 1/(2\alpha)\cdot\partial(p^{1/2}R_s)/\partial x_a = 1/(2\alpha)\cdot p^{1/2}\partial(p^{1/2}R_s)/\partial x_a$$
$$= 1/(2\alpha)\cdot p^{1/2}\cdot(x_p-x_s)/R_s\cdot\alpha/p$$
$$= \{1/(2p)\cdot\nabla x_p\}\cdot p/X \qquad \text{for (b)}$$
$$1/(2\alpha)\cdot\partial X/\partial x_a = 1/(2\alpha)\cdot\partial((pq/(p+q))^{1/2}R_{pq})/\partial x_a = 1/(2\alpha)\cdot(pq/(p+q))^{1/2}\partial(^2R_{sq})/\partial x_a$$
$$= 1/(2\alpha)\cdot(pq/(p+q))^{1/2}(x_p-x_q)/R_{pq}\cdot\alpha/p$$
$$= \{1/(2p)\cdot\nabla x_{pq}\}\cdot w/X \qquad \text{for (d)}$$
$$1/(2\gamma)\cdot\partial X/\partial x_c = 1/(2\gamma)\cdot\partial((pq/(p+q))^{1/2}R_{pq})/\partial x_c = 1/(2\gamma)\cdot(pq/(p+q))^{1/2}\partial(^2R_{sq})/\partial x_c$$
$$= 1/(2\gamma)\cdot(pq/(p+q))^{1/2}(x_p-x_q)/R_{pq}\cdot(-\gamma/q)$$
$$= \{-1/(2q)\cdot\nabla x_{pq}\}\cdot w/X \qquad \text{for (d)}$$

また、(b)(d)に対する FO(X) の一連の微分に対し、後の整理の都合上、次の関数を定義する。、

$$\mathrm{FOX} \equiv \partial F0(X)/\partial X = (\exp(-X2)-F0(X))/X$$
$$\mathrm{FOX3} \equiv X\cdot\partial(F0X/X)/\partial X = (-2X\exp(-X2)-3F0X)/X$$
$$\mathrm{FOX5} \equiv X^2\cdot\partial(F0X3/X^2)/\partial X = (4X^2\exp(-X2)-5F0X3)/X$$
$$\mathrm{FOX7} \equiv X^3\cdot\partial(F0X5/X^3)/\partial X = (-8X^3\exp(-X2)-7F0X3)/X$$
$$\mathrm{FOX9} \equiv X^4\cdot\partial(F0X7/X^4)/\partial X = (16X^4\exp(-X2)-9F0X3)/X$$

(ⅳ-5) F の微分

(a)(c)に対する微分$\partial F/\partial x_a$は、expBcd=1 であるから、

$$1/(2\alpha)\cdot\partial/\partial x_a\, F(x_a,Sb,Sc,Sd) = K\cdot 1/(2\alpha)\cdot\{(\partial/\partial x_a\, \mathrm{expAab})\cdot F0(X) + \mathrm{expAab}\cdot\partial/\partial x_a\, F0(X)\}$$
$$= K\cdot \mathrm{expAab}\cdot\{\,\angle x_a\,\} \qquad \text{for (a)}$$
$$1/(2\alpha)\cdot\partial/\partial x_a\, F(x_a,Sb,Sc,Sd) = K\cdot 1/(2\alpha)\cdot\{(\partial/\partial x_a\, \mathrm{expAab})\cdot F0(X) + \mathrm{expAab}\cdot\partial/\partial x_a\, F0(X)\}$$
$$= K\cdot \mathrm{expAab}\cdot\{\,\angle x_a\cdot F0(X) + 2\angle x_a\,\} \qquad \text{for (c)}$$
$$\equiv K\cdot \mathrm{expAab}\cdot\{\,\angle x_a\cdot F0(X) + \angle x_a\cdot F1(X)\} \qquad \text{for (c)}$$

ここに、

$$F1(X) \equiv \begin{cases} 0 & \text{for (a)} \\ 2 & \text{for (c)} \end{cases}$$

(b)(d)に対する微分$\partial F/\partial x_a$は、

$$(1/2\alpha)\cdot\partial/\partial x_a\, F(x_a,Sb,Sc,Sd)$$
$$= K\cdot(1/2\alpha)\cdot\{(\partial/\partial x_a\, \mathrm{expAab})\cdot \mathrm{expBcd}\cdot F0(X) + \mathrm{expAab}\cdot \mathrm{expBcd}\cdot\partial/\partial x_a\, F0(X)\}$$
$$= K\cdot \mathrm{expAab}\cdot \mathrm{expBcd}\cdot\{\,\angle x_a\cdot F0(X) + (1/2\alpha)\cdot\partial/\partial x_a\, F0(X)\}$$
$$= K\cdot \mathrm{expAab}\cdot \mathrm{expBcd}\cdot\{\,\angle x_a\cdot F0(X) + \partial F0(X)/\partial X\cdot(1/2\alpha)\partial X/\partial x_a\}$$
$$= K\cdot \mathrm{expAab}\cdot \mathrm{expBcd}\cdot\{\,\angle x_a\cdot F0(X) + \partial F0(X)/\partial X\cdot(1/2\alpha)\partial X/\partial x_a\}$$
$$= K\cdot \mathrm{expAab}\cdot \mathrm{expBcd}\cdot\{\,\angle x_a\cdot F0(X) + \mathrm{FOX}\cdot(1/2\alpha)\partial X/\partial x_a\}$$
$$= \begin{cases} K\cdot \mathrm{expAab}\cdot \mathrm{expBcd}\cdot\{\,\angle x_a\cdot F0 + \{(1/2p)\cdot\nabla x_p\,\}\cdot p\cdot \mathrm{FOX}/X\} & \text{for (b)} \\ K\cdot \mathrm{expAab}\cdot \mathrm{expBcd}\cdot\{\,\angle x_a\cdot F0 + \{(1/2p)\cdot\nabla x_{pq}\,\}\cdot w\cdot \mathrm{FOX}/X\} & \text{for (d)} \end{cases}$$
$$\equiv \begin{cases} K\cdot \mathrm{expAab}\cdot \mathrm{expBcd}\cdot\{\,\angle x_a\cdot F0 + \{(1/2p)\cdot\nabla x_p\,\}\cdot F1(X)\} & \text{for (b)} \\ K\cdot \mathrm{expAab}\cdot \mathrm{expBcd}\cdot\{\,\angle x_a\cdot F0 + \{(1/2p)\cdot\nabla x_{pq}\,\}\cdot F1(X)\} & \text{for (d)} \end{cases}$$

ここに、

$$F1(X) \equiv \begin{cases} p\cdot \mathrm{FOX}/X & \text{for (b)} \\ w\cdot \mathrm{FOX}/X & \text{for (d)} \end{cases}$$

更に、続けると、{　　}

$$(1/2\alpha)\cdot\partial/\partial x_a\, F1(X) = (1/2\alpha)\cdot\{p\cdot\partial/\partial x_a\, \mathrm{FOX}/X\}$$
$$= p\cdot\partial/\partial X\, \mathrm{FOX}/X\cdot\{(1/2\alpha)\cdot\partial X/\partial x_a\} = p\cdot\partial/\partial X\, \mathrm{FOX}/X\cdot\{(1/2p)\cdot\nabla x_p\cdot p/X\}$$
$$= \{(1/2p)\cdot\nabla x_p\}\cdot p^2\cdot\{1/X\cdot\partial(\mathrm{FOX}/X)/\partial X\}$$
$$= \{(1/2p)\cdot\nabla x_p\}\cdot p^2\cdot \mathrm{FOX3}/X^2 \qquad \equiv (1/2p)\cdot\nabla x_p\cdot F2(X)$$
$$(1/2\alpha)\cdot\partial/\partial x_a\, F1(X) = (1/2\alpha)\cdot\{w\cdot\partial/\partial x_a\, \mathrm{FOX}/X\}$$
$$= w\cdot\partial/\partial X\, \mathrm{FOX}/X\cdot\{(1/2\alpha)\cdot\partial X/\partial x_a\} = w\cdot\partial/\partial X\, \mathrm{FOX}/X\cdot\{(1/2p)\cdot\nabla x_{pq}\cdot w/X\}$$
$$= \{(1/2p)\cdot\nabla x_{pq}\}\cdot w^2\cdot\{1/X\cdot\partial(\mathrm{FOX}/X)/\partial X\}$$
$$= \{(1/2p)\cdot\nabla x_{pq}\}\cdot w^2\cdot \mathrm{FOX3}/X^2 \qquad \equiv (1/2p)\cdot\nabla x_{pq}\cdot F2(X)$$
$$(1/2\beta)\cdot\partial/\partial x_b\, F1(X) = (1/2\beta)\cdot w\cdot\partial/\partial x_b\, \mathrm{FOX}/X\}$$
$$= \{(-1/2q)\cdot\nabla x_{pq}\}\cdot w^2\cdot \mathrm{FOX3}/X^2 \qquad \equiv (-1/2q)\cdot\nabla x_{pq}\cdot F2(X)$$

すなわち､原子 a～d の各々の s 軌道でない軌道の x，y，z の数を ka～kd (n=ka+kb+kc+kd)として、

$$Fn(X) \equiv \begin{cases} p^n\cdot \mathrm{FOX}(2n-1)/X^n & \text{for (b)} \\ w^n\cdot \mathrm{FOX}(2n-1)/X^n & \text{for (d)} \end{cases}$$

（v）全体整理

これまでの微分操作をまとめると以下の表の如きになり、その値を Ta,Tb,Tc,Td とすると、

F(a,b)= K・expAab・Σ(TaTb)　　　　　　　　(ex Σ(TaTb)= ⊿x_a⊿x_b F0)

F(a,b,c,d)= K・expAab・expBcd・Σ(TaTbTcTd)　(ex Σ(TaTbTcTd)= ⊿x_a(1/(2p))(-▽x_{pq}/(2q)) F2)

	(1/2α)・∂/∂x_a	(1/2β)∂/∂x_b	(1/2γ)・∂/∂x_c	(1/2δ)∂/∂x_d	(1/2α)・∂/∂y_a
exp(−sR_{ab}^2)	⊿x_a	⊿x_b	―	―	⊿y_a
exp(−tR_{cd}^2)	0	0	⊿x_c	⊿x_d	0
⊿x_a	1/(2p)−1/(2α)	1/2p	0	0	0
▽x_p	1/(2p)	同左	0	0	0
▽x_{pq}	1/(2p)	同左	-1/2q	-1/2q	0
F0(3-2sR_{ab}^2)	(⊿x_a)・2	(⊿x_b)・2	―	―	(⊿y_a)・2
Fn($p^{1/2}R_s$)	(▽x_p/(2p))Fn+1	同左	―	―	(▽y_p/(2p))Fn+1
Fn($w^{1/2}R_{pq}$)	(▽x_{pq}/(2p))Fn+1	同左	(-▽x_{pq}/(2q))Fn+1	同左	(▽y_{pq}/(2p))Fn+1

（v-1）重なり積分（ F0＝1 、F1＝0 ）

(Sa,Sb)　　　　　　　　　　　　＝1

(x_a,Sb) = 1/(2α)・{ ∂/∂x_a (Sa,Sb) }　　＝ ⊿x_a　　　　---------- ∂/∂x_a expAab

(x_a,x_b) = 1/(2β)・{ ∂/∂x_b (x_a,Sb)} }　　＝ ⊿x_a ⊿x_b　　　　---------- ∂/∂x_b expAab

(x_a,y_b) = 1/(2β)・{ ∂/∂y_b (x_a,Sb)} }　　＝ ⊿x_a ⊿y_b　　　　---------- ∂/∂y_b expAab

(x_a^2,Sb) = 1/(2α)・{ ∂/∂x_a (x_a,Sb) + (Sa,Sb) } = ⊿x_a ⊿x_a −{1/ (2p)−1/(2α)} + 1/(2α)

＝ ⊿x_a ⊿x_a +1/(2p)

（v-2）コア積分２（ F0＝3−2sR_{ab}^2 、F1＝2 ）

＜Sa,Sb＞　　　　　　　　　　＝F0

＜x_a,Sb＞= 1/(2α)・{ ∂/∂x_a〔Sa,Sb〕} = (F0)・⊿x_a　　　　---------- ∂/∂x_a expAab

＋ ⊿x_a・F1　　　　---------- ∂/∂x_a F0

＜x_a,x_b＞= 1/(2β)・{ ∂/∂x_b〔x_a,Sb〕} = (⊿x_aF0+⊿x_aF1)・⊿x_b　　　　---------- ∂/∂x_b expAab

+1/(2p)・F0+1/(2p)・F1　　　　---------- ∂/∂x_b⊿x_a

+⊿x_a・(⊿x_b・F1)　　　　---------- ∂/∂x_b F0

＜x_a,y_b＞= 1/(2β)・{ ∂/∂y_b〔x_a,Sb〕} = (⊿x_aF0+⊿x_a F1)・⊿y_b　　　　---------- ∂/∂y_b expAab

+ 0　　　　---------- ∂/∂y_b⊿x_a

+⊿x_a・⊿y_b・F1　　　　---------- ∂/∂y_b F0

＜x_a^2,Sb＞= 1/(2α)・{ ∂/∂x_b〔x_a,Sb〕+〔Sa,Sb〕}

=(⊿x_aF0+⊿x_a F1)・⊿x_a　　　　---------- ∂/∂x_a expAab

−{1/ (2p)−1/(2α)}・F0+{1/ (2p)−1/(2α)}・F1 ---- ∂/∂x_a⊿x_a

+⊿x_a・⊿x_a・F1　　　　---------- ∂/∂x_a F0

+1/(2α)・F0　　　　---------- 1/(2α)・〔Sa,Sb〕

＝ ⊿x_a⊿x_a・F0+⊿x_a⊿x_a F1

+{1/ (2p)−1/(2α)}・F1

+ ⊿x_a・⊿x_a・F1

+ 1/(2p)・F0

（ｖ-3）コア積分１　（ $F0 = F0(p^{1/2}R_s)$ 、$Fn = p^n$・$FOX(2n-1)/X^n$ ）

〔Sa,Sb〕＝F0

〔x_a,Sb〕＝1/(2α)・{ ∂/∂x_a〔Sa,Sb〕}

= (F0)・$\angle x_a$ --------- ∂/∂x_a expAab

+(1/(2p)・∇x_p)・F1 --------- ∂/∂x_a F0

= $\angle x_a$ F0 + 1/(2p)∇x_p F1

〔x_a,x_b〕＝1/(2β)・{ ∂/∂x_b〔x_a,Sb〕}

=($\angle x_a$・F0+(1/(2p)・∇x_p)・F1)・$\angle x_b$ --------- ∂/∂x_b expAab

+ F0・1/(2p) --------- ∂/∂x_b $\angle x_a$

+1/(2p)・1/(2p)・F1 --------- ∂/∂x_b ∇x_p

+$\angle x_a$・(1/(2p)・∇x_p・F1) --------- ∂/∂x_b F0

+1/(2p)∇x_p・(1/(2p)∇x_p F2) --------- ∂/∂x_b F1

= {$\angle x_a \angle x_b$ +1/(2p) } F0 + { 1/(2p)$\nabla x_p \angle x_b$+$\angle x_a$・1/(2p)∇x_p ・1/(2p) ・1/(2p)} F1

+ 1/(2p)∇x_p(1/(2p)∇x_p F2

〔x_a,y_b〕＝1/(2β)・{ ∂/∂y_b〔x_a,Sb〕}

=($\angle x_a$・F0+(1/(2p)・∇x_p)・F1)・$\angle y_b$ --------- ∂/∂y_b expAab

+ 0 --------- ∂/∂y_b $\angle x_a$

+0 --------- ∂/∂y_b ∇x_p

+$\angle x_a$・(1/(2p)・∇y_p・F1) --------- ∂/∂y_b F0

+1/(2p)∇x_p・(1/(2p)∇y_p F2) --------- ∂/∂y_b F1

= {$\angle x_a \angle y_b$ } F0 + { 1/(2p)$\nabla x_p \angle y_b$+$\angle x_a$・1/(2p)∇y_p} F1+ 1/(2p)∇x_p(1/(2p)∇y_p F2

〔x_a^2, Sb〕＝1/(2α)・{ ∂/∂x_a〔x_a,Sb〕+〔Sa,Sb〕}

=($\angle x_a$・F0+(1/(2p)・∇x_p)・F1)・$\angle x_a$ --------- ∂/∂x_b expAab

+ {1/ (2p)－1/(2α)}・F0 --------- ∂/∂x_b $\angle x_a$

+1/(2p)・1/(2p)・F1 --------- ∂/∂x_a ∇x_p

+$\angle x_a$・(1/(2p)・∇x_p・F1) --------- ∂/∂x_a F0

+1/(2p)∇x_p・(1/(2p)∇x_p F2) --------- ∂/∂x_a F1

+ 1/(2α)・F0 -------- 1/(2α)・〔Sa,Sb〕

= {$\angle x_a \angle x_a$ +1/(2p) } F0 + {2$\angle x_a$・1/(2p)∇x_p+1/(2p)・1/(2p) } F1+ 1/(2p)∇x_p(1/(2p)∇x_p F2

（ｖ-4）交換積分（$F0=F0(pq/(p+q)^{1/2}R_{pq})$,$Fn = w^n$・$FOX(2n-1)/X^n$ ）

同様の操作を行えば、以下の如くにもとめられる。

(Sa,Sb｜Sc,Sd) = F0

(x_a,x_a｜Sc,Sd) = $\angle x_a$F0 + 1/(2p)∇x_{pq} F1

(x_a,y_b｜Sc,Sd) = $\angle x_a \angle y_b$ F0 + {$\angle x_a$・1/(2p)∇y_{pq}+1/(2p)$\nabla x_{pq} \angle y_b$} F1+ 1/(2p)∇x_p(1/(2p)∇x_p F2

(x_a,Sb｜x_a ,Sd) =$\angle x_a \angle x_c$ F0 + {$\angle x_a$・1/(2q)∇x_{pq}+1/(2p)$\nabla x_{pq} \angle x_c$+1/(2p)(－1/(2q)) } F1

+ 1/(2p)∇x_{pq}(1/(2q)∇x_{pq} F2