分子積分に関するプログラミングの研究 I

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A Study of programming of Molecular Integrals in the Electronic Emputer I.

—— Programming of auxiliary functions ——

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If one attacks the quantum mechanical problems of molecular structure by an expansion of the wave function's in terms of AO's (atomic orbitals), then the differential equation's are reduced to matrix equations and the difficulties conceutrate to a large extent in the evaluation of the integrals in terms of which the matrix element are defined.

If we use Slater type AO's, then all the integrals, in volving only two centers can be obtained in closed analytical form (except for one tyne, two-center exchange integrals).

These two-center integrals are then only ones, occurring in diatomic molecules, and also the most important one occurring in polyatomic molecules.

We obtained the programs of the awxiliary functions in molecular integrals by Algol's expression which are used in the electronic computer of FACOM 202 (the Instilute of Sobid State Physics, Jokyo University).

分子積分を求めるに色々の方法があるがここでは小谷方法に準拠して求めた。そして，まず分子積分に必要な補助函数の計算をＡＬＧＯＬによるプログラムでつくった。

§ 1　補助函数の定義
§ 2　補助函数の計算の手順
§ 3　プログラム (ALGOL's Expression)
§ 4　謝　　辞

§ 1　補助函数の定義

$$A_n(\alpha)=\int_1^{\infty} e^{-\alpha\lambda}\lambda^n d\lambda$$

$$B_n(\beta)=\int_{-1}^{1} e^{-\beta\mu}\mu^n d\mu$$

$$E_i(\alpha)=\int_{-\infty}^{\alpha} \frac{e^x}{x} dx$$

$$-E_i(-\alpha)=\int_{\alpha}^{\infty} \frac{e^{-x}}{x} dx$$

$$f_\tau(m,\alpha)=\int_1^{\infty} Q_\tau(x)e^{-\alpha x}x^m dx$$

$$S_\tau(m.\ n : \alpha, \beta)=\int_1^{\infty} Q_\tau(x)e^{-\alpha x}x^m dx\int_1^{\alpha} e^{-\beta y}y^n dy$$

$$W^{\nu}_{\tau}(m, n\,; \alpha\beta) = \int_1^\infty \int_1^\infty Q^{\nu}_{\tau}(\lambda>) P^{\nu}_{\tau}(\lambda<) e^{-\alpha\lambda_1 - \beta\lambda_2} \lambda_1{}^m \lambda_2{}^n \times (\lambda_1{}^2-1)^{\frac{\nu}{2}} (\lambda_2{}^2-1)^{\frac{\nu}{2}} d\lambda_1 d\lambda_2$$

§ 2　補助函数の計算の手順

$A_n(\alpha)$:

$$A_0(\alpha) = \frac{e^{-\alpha}}{\alpha}$$

$$A_1(\alpha) = \frac{e^{-\alpha}}{\alpha}\left(1 + \frac{1}{\alpha}\right)$$

$$A_2(\alpha) = \frac{e^{-\alpha}}{\alpha}\left\{\left(1 + \frac{1}{\alpha}\right)\frac{2}{\alpha} + 1\right\}$$

$$A_3(\alpha) = \frac{e^{-\alpha}}{\alpha}\left[\left\{\left(+1\,\frac{1}{\alpha}\right)\frac{2}{\alpha} + 1\right\}\frac{3}{\alpha} + 1\right]$$

…………………

$n=0$: $W=1$

$n=1$: $\frac{1}{\alpha}+1$

$n=2$: $\left(\frac{1}{\alpha}+1\right)\frac{2}{\alpha}+1$

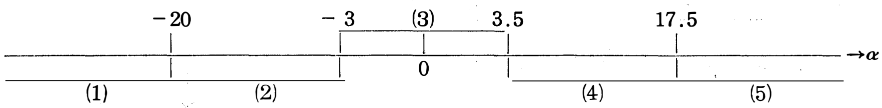
$n=3$: $\left\{\left(\frac{1}{\alpha}+1\right)\frac{2}{\alpha}+1\right\}\frac{3}{\alpha}+1$

…………………

$B_n(\alpha)$:

$B_n(\beta) = -A_n(\beta) - (-1)^n A_n(-\beta)$を用いる。

$\left.\begin{matrix} E_i(\alpha) \\ -E_i(-\alpha) \end{matrix}\right\}$:



(1)　$-E_i(-\alpha) = \frac{e^{-\alpha}}{\alpha}\left\{1 - \frac{1!}{\alpha} + \frac{2!}{\alpha_2} - \frac{3!}{\alpha_3} + \cdots\cdots\right\}$

(2)　$-\{E_i(-\alpha-\triangle\alpha) - E_i(-\alpha)\} = e^{-\alpha}\frac{\triangle\alpha}{\alpha}\left[\sum_{r=0}^{\infty}\left(\frac{\triangle\alpha}{\alpha}\right)^r\left\{\frac{r!}{(\triangle\alpha)^{r+1}} - A\nu(\triangle\alpha)\right\}\right]$

(3)　$0 \sim 3.5$　$E_i(\alpha) = C + \log\alpha + \frac{\alpha}{1.1!} + \frac{\alpha^2}{2.2!} + \frac{\alpha^3}{3.3!} + \cdots\cdots$

$-3 \sim 0$　$-E_i(-\alpha) = -C - \log(-\alpha) + \frac{\alpha}{1.1} - \frac{\alpha^2}{2.2!} + \frac{\alpha^3}{3.3!}\cdots\cdots$

(4)　$E_i(\alpha+\triangle\alpha) - E_i(\alpha+\triangle\alpha) - E_i(\alpha) = \frac{e^{\alpha+\triangle\alpha}}{\alpha+\triangle\alpha}\triangle\alpha\left[\sum_{r=0}^{\infty}\left(\frac{\triangle\alpha}{\alpha+\triangle\alpha}\right)^r\left\{\frac{r!}{(\alpha\triangle)^{r+1}} - A_r(\triangle\alpha)\right\}\right]$

(5)　$E_i(\alpha) = \frac{e^{\alpha}}{\alpha}\left\{1 + \frac{1!}{\alpha} + \frac{2!}{\alpha^2} + \frac{3!}{\alpha^2} + \cdots\cdots\right\}$

$$f_\tau(m,\alpha) = \int_1^\infty Q_\tau(x) e^{-dx} x^m dx$$

漸化式は

$$f_1(m+2,\alpha) = f^1(m,\alpha) + \frac{1}{\alpha}\{2f_1(m+1,\alpha) - A_m + (\alpha)\} + \frac{m+1}{\alpha}\{f_1(m+1,\alpha) - f_1(m-1,\alpha)\}$$

$$= f_1(m,\alpha) + \frac{1}{\alpha}[3f_1(m+1,\alpha) - f_0(m+1,\alpha) - f_0(m,\alpha) + m\{f_1(m+1,\alpha)f(m-1,\alpha)\}]$$

具体的に展開すると，

$m=0\quad f_1(2,\alpha)=f_1(0,\alpha)+\dfrac{1}{\alpha}[3f_1(1,\alpha)\qquad -f_0(0,\alpha)]$

$m=1\quad f_1(3,\alpha)=f_1(1,\alpha)+\dfrac{1}{\alpha}[4f_1(2,\alpha)-f_1(o,\alpha)-f_0(1,\alpha)]$

$m=2\quad f_1(4,\alpha)=f_1(2,\alpha)+\dfrac{1}{\alpha}[5f_1(3,\alpha)-2f_1(1,\alpha)-f_0(2,\alpha)]$

ただし　$f_0(0,\alpha)=f_0(2,\alpha)-\dfrac{1}{\alpha}[2f_0(1,\alpha)-A_0(\alpha)]$

$$=\frac{1}{2\alpha}e^{-\alpha}[c+\log 2\alpha+e^{2\alpha}\{-E_i(-2\alpha)\}]$$

$$f_1(0,\alpha)=\frac{1}{2}[(c+\log 2\alpha)A_1(\alpha)+(-E_i(-2\alpha))\{A_1(\alpha)+\beta_1(\alpha)\}]-Ao(\alpha)$$

$$f_1(1,\alpha)=\frac{1}{2}[(c+\log 2\alpha)A_2(\alpha)+(-E_i(-2\alpha))\{A_2(\alpha)+\beta_2(\alpha)\}]-A_1(\alpha)-\frac{A_0(\alpha)}{\alpha}$$

また　$f_0(m,\alpha)=f_1(m-1,\alpha)+A_{m-1}(\alpha)$

具体的に展開すると，

$m=0\quad fo(1,\alpha)=f_1(0,\alpha)+A_0(\alpha)$

$m=1\quad f_0(2,\alpha)=f_1(1,\alpha)+A_1(\alpha)$

………………

$f_0(0,\alpha)$，$f_1(0,\alpha)$，$f_1(1,\alpha)$ はそれぞれ別個に計算で出し，下図の順序で進める。
□ 内の数値が与えられたものとして初め ⟶ の方向に計算をし，次は ………→ の方向に計算を進める。
このように左右を交互にくり返し，μ の数を増しながら以下の計算を実行する。

$\boxed{\text{数値0をおく}}$

$n=0\quad \boxed{f_0(0,\alpha)}\quad \cdots\cdots\cdots\cdots \boxed{f_1(0,\alpha)}=F_0$

$1\quad f_0(1,\alpha)=f_1(1,\alpha)+A_0(\alpha)\quad \boxed{f_1(0,\alpha)}=F_1$

$2\quad f_0(2,\alpha)=f_1(1,\alpha)+A_1(\alpha),\ f_1(2,\alpha)=f_1(0,\alpha)+\dfrac{1}{\alpha}[3f_1(1,\alpha)\qquad -f_0(0,\alpha]$

$3\quad f_0(3,\alpha)=f_1(2,\alpha)+A_2(\alpha),\ f_1(3,\alpha)=f_1(1,\alpha)+\dfrac{1}{\alpha}[4f_1(2,\alpha)-f_1(0,\alpha)-f_0(1,\alpha)]$

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E[i]　A[i]　F[i]　J　K

S. W. Z :

$S_0(n,m:\beta\alpha)$

$\alpha S_0(n,m:\beta\alpha)=mS_0(n,m-1:\beta\alpha)+e^{-\alpha}f_0(n,\beta)-f_0(m+n:\alpha+\beta)$

$m=0\quad n=0\quad \alpha S_0(00:\beta\alpha)=\qquad +e^{-\alpha}f_0(0,\beta)-f_0(0:\alpha+\beta)$

$1\quad \alpha S_0(1,0:\beta\alpha)=\qquad +e^{-\alpha}f_0(1,\beta)-f_0(1:\alpha+\beta)$

$2\quad \alpha S_0(2,0:\beta\alpha)=\qquad +e^{-\alpha}f_0(2,\beta)-f_0(2:\alpha+\beta)$

………………

$m=1\quad n=0\quad \alpha S_0(0,1:\beta\alpha)=S_0(00:\beta\alpha)\ +e^{-\alpha}f_0(0,\beta)-f_0(1:\alpha+\beta)$

$1\quad \alpha S_0(1,1:\beta\alpha)=S_0(1,0:\beta\alpha)+e^{-\alpha}f_0(1,\beta)-f_0(2:\alpha+\beta)$

$2\quad \alpha S_0(2,1:\beta\alpha)=S_0(2,0:\beta\alpha)+e^{-\alpha}f_0(2,\beta)-f_0(3:\alpha+\beta)$

………………

$m=2\quad n=0\quad \alpha S_0(0,2:\beta\alpha)\Sigma 2S_0(0,1:\beta\alpha)+e^{-\alpha}f_0(0,\beta)-f_0(2:\alpha+\beta)$

1 $\alpha S_0(1,2:\beta\alpha)=2S_0(1,1:\beta\alpha)+e^{-\alpha}f_0(1,\beta)-f_0(3:\alpha+\beta)$

2 $\alpha S_0(2,2:\beta\alpha)=2S_0(2,2:\beta\alpha)+e^{-\alpha}f_0(2,\beta)-f_0(4:\alpha+\beta)$

....

$S_1(n,m+1:\beta\alpha)$

$\alpha S_1(n,m+1:\beta\alpha)=m+1)S_1(n,m=\beta\alpha)+e^{-\alpha}f_1(m+n+1:\alpha+\beta)$

m=−1 n=0 $\alpha S_1(0,0:\beta\alpha)=\quad e^{-\alpha}f_1(0,\beta)-f_1(0:\alpha+\beta)$

1 $\alpha S_1(0,1:\beta\alpha)=\quad e^{-\alpha}f_1(1,\beta)-f_1(1:\alpha+\beta)$

2 $\alpha S_1(0,2:\beta\alpha)=\quad e^{-\alpha}f_1(2,\beta)-f_1(2:\alpha+\beta)$

....

m=0 n=0 $\alpha S_1(0,1:\beta\alpha)=S_1(0,0:\beta\alpha)+e^{-\alpha}f_1(0,\beta)-f_1(1:\alpha+\beta)$

1 $\alpha S_1(1,1:\beta\alpha)=S_1(1:0:\beta\alpha)+e^{-\alpha}f_1(1,\beta)-f_1(2:\alpha+\beta)$

2 $\alpha S_1(2,1:\beta\alpha)=S_1(2,0:\beta\alpha)+e^{-\alpha}f_1(2,\beta)-f_1(3:\alpha+\beta)$

....

$S_0(m,n:\alpha\beta)$

$\beta S(m,n:\alpha\beta)=nS_0(m,n-1:\alpha\beta)+e^{-}{}_{\beta}f_0(m,\alpha)-f_0(m+n=\alpha+\beta)$

m=0 n=0 $\beta S_0(0,1:\alpha\beta)=\quad e^{-\beta}f_0(0,\alpha)-f_0(0:\alpha+\beta)$

1 $\beta S_0(0,1:\alpha\beta)=S_0(0,0:\alpha\beta)+e^{-\beta}f_0(0,\alpha)-f_0(1:\alpha+\beta)$

2 $\beta S_0(0,2:\alpha\beta)=2S_0(0,1:\alpha\beta)+e^{-\beta}f_0(0,\alpha)-f_0(2:\alpha+\beta)$

....

m=1 n=0 $\beta S_0(1,0:\alpha\beta)=\quad e^{-\beta}f_0(1,\alpha)-f_0(1:\alpha+\beta)$

1 $\beta S_0(1,1:\alpha\beta)=S_0(1,0:\alpha\beta)+e^{-\beta}f_0(1,\alpha)-f_0(2:\alpha+\beta)$

2 $\beta S_0(1,2:\alpha\beta)=2S_0(1,1:\alpha\beta)+e^{-\beta}f_0(1,\alpha)-f_0(3:\alpha+\beta)$

....

m=2 n=0 $\beta S_0(2,0:\alpha\beta)=\quad e^{-\beta}f_0(2,\alpha)-f_0(2:\alpha+\beta)$

1 $\beta S_0(2,1:\alpha\beta)=S_0(2,0:\alpha\beta)+e^{-\beta}f_0(2,\alpha)-f_0(3:\alpha+\beta)$

2 $\beta S_0(2,2:\alpha\beta)=2S_0(2,1:\alpha\beta)+e^{-\beta}f_0(2,\alpha)-f_0(4:\alpha+\beta)$

....

$S_1(m,n+1:\alpha\beta)$

$\beta S_1(m,n+1:\alpha\beta)=(n+1)S_1(m,n:\alpha\beta)+e^{-\beta}f_1(m:\alpha)-f_1(m+n+1:\alpha+\beta)$

式の記号化：

$\alpha S_1(n,m+1:\beta\alpha)=m+1)S_1(n,m:\beta\alpha)+e^{-\alpha}f_1(n,\beta)-f_1(m+n+1:\alpha+\beta)$ ....(1)

X S1BA[i:j+1] (j+1)S1BA[i,j] exp(−X)F1B[i] F1[i+j+1]

$\alpha S_0(n,m:\beta\alpha)=mS_0(n,m-1:\beta\alpha)+e^{-\alpha}f_0(n,\beta)-f_0(m+n:\alpha+\beta)$ ....(2)

X S0BA[i,j] j S0BA[i,j−1] exp(−X)F0B[i] F0[i+j]

$\beta S_1(m,n+1:\alpha\beta)=n+1)S_1(m,n:\alpha\beta)+e^{-\beta}f_1(m,\alpha)-f_1(m+n+1:\alpha+\beta)$ ....(3)

Y S1AB[j,i+1] (i+1) S1AB[j,i] exp(−Y)F1A[j] F1[i+j+1]

$\beta S_0(m,n:\alpha\beta)=nS_0(m,n-1:\alpha\beta)+e^{-\beta}fom,\alpha)-f_0(m+n:\alpha+\beta)$ ....(4)

Y S0AB[j,i] i S0AB[j,i−1] exp(−Y)F0A[j] F0[i+j]

$W_0{}^0(m,n:\alpha\beta)=S_0(m,n:\alpha\beta)+S_0(n,m:\beta\alpha)$ ....(5)

W_0[j,i] S0AB[j,i] S0BA[i,j]

$W_1{}^0(m,n:\alpha\beta)=S_1(m,n+1:\alpha\beta)+S_1(n,m+1:\beta\alpha)$ ....(6)

W1[j,i] S1AB[j,i+1] S1BA[i,j+1]

$Z_0(m,n:\alpha\beta)=S_0(m,n+1:\alpha\beta)+S_0(n,m+2:\beta\alpha)+S_1(m+1,n:\alpha\beta)+S_1(n+1,m:\beta\alpha)$

$+3W^0{}_1(m+1,n+1:\alpha\beta)$ ....(7)

ZO[j,i] S0AB[j,i+2] S0BA[i,j+2] S1AB[j+1,i] S1BA[i+j,1]

3※W1[j+1,i+1]

$4W_2^0(m,n:\alpha\beta)=W_0^0(m,n:\alpha\beta)-3Z_0(m,n:\alpha\beta)$ ··························(8)

4 ⁎W 2〔j,i〕　　W0〔j,i〕　　3 ⁎ZO〔j,i〕

$Z_1(m,n:\alpha\beta)=3W^0{}_1(m+2,n:\alpha\beta)+3W_1^0(m+2,n:\alpha\beta)-W_0^0(m+1,n+1:\alpha\beta)$

$-W^0{}_1(m,n:\alpha\beta)-5W_2^0(m+1,n+1:\alpha\beta)$ ··························(9)

Z1〔j,i〕　　3 ⁎W 1〔j,i+2〕　　3 ⁎W1〔j+2,i〕　　WO〔j+1,i+1〕

W 1〔j,i〕　　5 ⁎W 2〔j+1,i+1〕

$9W_3^0(m,n:\alpha\beta)=4W_1^0(m,n:\alpha\beta)-5Z_1(m,n:\alpha\beta)$ ··························(10)

9 ⁎W 3〔j,i〕　　4 ⁎W 1〔j,i〕　　5 ⁎Z 1〔j,i〕

§ 3　プログラム

Algol プログラム Ⅰ：

```
                          An                Bn
↓begin  ↓integer n ;
        ↓real    Y ;
        ↓array  A, B, C, D〔0:15〕;
        ↓procedure layout (X,M) ;
        ↓Value  X ;  ↓real X ;  ↓array M ;
        ↓begin  ↓integer n ;
                ↓real  W;W:=1 ;
                ↓for   n : =0  ↓step 1  ↓until 15  ↓do
                      ↓begin
                          W:=W⁎n⁎X+1 ;
                          M〔n〕:=exp(-1/X)⁎X⁎W ;
                          crlf ;
                          printinteger  (2,n) ;
                          Printreal     (10,M〔n〕)
                      ↓end
        ↓end ;
          readreal (Y) ;
            lagout (1/Y, A) ;
          readreal (Y) ;
            layout (1/Y, B) ;
          readreal (Y)
            layout (1/r,C) ;
               E :=-1
        ↓for  n:=0   ↓step 1  ↓until 15  ↓ do
                ↓begin
                        E:=E⁎(-1) ;
                        D〔n〕:=-B〔n〕-E⁎C〔n〕 ;
                        crlf ;
                        Printinteger (2, n) ;
                        printreal    (10, M〔n〕) ;
                ↓end ;
        ↓end ;
```

Algol プログラム Ⅱ：

```
                 Ei(x),          -Ei(-x)
↓begin  ↓integer j,  n ;
        ↓real  k, a, c, d, w, h, t, u, v, x, y, e, z ;
         readreal (x) ;
        ↓if  x≧-20 ∨ 17.5<x  ↓then
E1:     ↓begin
            c:=h:=1  ;  u:=1/x ;
          ↓for n:=1, n+1   ↓ while  h≤  10-11  ↓do
            ↓begin  h:=h×n×u ;  c:=c+h  ↓end ;
                e:=u×c×exp(x)
        ↓end ;
        ↓else  ↓if  -3<x & x≤3.5  ↓then
E3:     ↓begin
          c:=0  ;  h:=u:=1  ;
            ↓for n:=1, n+1  ↓while  u≤10^-11  ↓do
              ↓begin  h:=h×x/n ;  u:=h/n ;  c:=c+u  ↓end ;
           e:=↓if  x=0  ↓then  -0.5772156649  ↓else  ↓if  x>0  ↓then
               c+ln(x)+0.5772156649  ↓else-c-ln(-x)-0.5772156649
        ↓end
        ↓else
E2:     ↓begin  n:=if  x<0  ↓then 33  ↓else 27 ;
                cref ; printstring ('call  array B') ; printinteger (2, n) ;
                halt (NEXT) ;
NEXT:           ↓begin  ↓array B [o:n) ;
                        READARRAY1 (1, B) ;
                        ↓if  x<0  ↓then
                          ↓begin
                             n:=entier (cabs(x)-3)/0.5) ;  k:=x+0.5×n ;
                             v:=abs (1/(x-k)) ;  z:=-v
                          ↓end
                          ↓else
E4:                       ↓begin
                             n:=entier((x-3.5)/0.5) ;  k:=x-0.5×n ;  z:v:=1/x
                          ↓end
E5:              h:=y:=c:=d:=1 ;
                 ↓if  abs (k)>10^-11)  ↓then
                   ↓begin
                     t:=1/k ;  u:=t-exp(-k)×t ;
                     ↓for  j:=1, j+1   ↓while  h>10^-11  ↓do
                                ↓begin
                                  h:=h×v×k ;  c:=j×c ;  y:=y×v ;  d:=d×j×t+1 ;
                                  a:=exp(-k)×t×d ;  u:=y×t×c-a×h+u
                                ↓end ;
                           e:=B[n]+exp(1/v)×z/t×u
```

```
                    ↓end  ↓elfee:=β[n]
                 ↓end
            ↓end ;
          crlf ;  printstring(‘x=’) ;  printreal (10, x) ;
                  printstring(‘e=’) ;  printreal (10, e) ;
      ↓end
```

Algol プログラム Ⅲ :

```
              F0                F1
↓begin  ↓integer n ;
         readinteger(n) ;
        ↓begin  ↓integer  J, k ;  ↓veal  X, F10, F11, F00, D ;
                ↓arrauy  A[0:n], F1[-1:n], F0[1:n+1] ;
              ↓procedure layout (X, F10, F11, F00) ;
                        ↓value  X, F10, F11, F00 ;
                        ↓real   X, F10, F11, F00 ;
                ↓begin  ↓integer  i ;
                        D:1 ;  J:=3 ;  K:=0 ;
                        F0[0]:=F00, F1[0]:=F10, F1[1]:=F11 ;  F1[-1]:=0 ;
                        ↓for  i:=0  ↓step 1  ↓until n  ↓do
                        ↓begin
                            D:=D×i×X+1 ;  A[i]:=exp(-1/x)×X×D ;
                            F0[i+1]:=F1[i]+A[i] ;
                            F1[i+2]:=F1[i]+X×(J×F1[i+1]-K×[i-1]-F0[i]) ;
                            K:=K+1;  J:=J+1;  crlf ;
                            printinteger (2, i) ;
                            printreal    (10,F0[i+1]) ;
                            printreal    (10,F1[i+2])
                        ↓end
                ↓end ;
                        READREAL 4  (4, Y, F10, F11, F00) ;
                          lagout     (1/Y, F10, F11, F00) ;
                        READREAL 4  (4, Y, F10, F11, F00) ;
                          lagout     (1/Y, F10, F11, F00) ;
                        READREAL 4  (4, Y, F10, F11, F00) ;
                          lagout     (1/Y, F10, F11, F00) ;
        ↓end
↓end ;
```

Algol プログラム Ⅳ :

```
              S.   W.   Z.
↓begin  ↓integer  n, i, j, k, l, I, J ;
  readinteger (n) ;
        ↓begin  ↓real  X, Y, C, D, K, L ;
                ↓array  S0ba, S0ab[0:n, -1:n], S1ba, S1ab[0:n, -I:n+1],
```

```
            f1a, f1b, f0a, f0b [0:n], f0[0:n+n], f1[0:n+n],
            M, W0, W1[0:n, 0:h], Z0, W2[0:n-2, 0:n-2],
            Z1, W3[0:n-3, 0:n-3] ;
    ↓procedure PRLNT(N, n, M) ;
    ↓Value n;  ↓integer n ;  ↓string N ;  ↓array M ;
    ↓begin  ↓integer i, j, k, l ;
       printstring (N) ;  cr ;
       ↓for  j:=0  ↓step 1  ↓until n  ↓ do
         ↓begin printstring ('j=') ;  printinteger (2,j);  l:=n+1 ; i:=-1 ;
           [1:  ↓for  K:=1  ↓step 1  ↓until 7  ↓do
             ↓begin l:=l-1 ; i:=i+1 ; printreal(10,M[i,j]); space(1);
               ↓if  l=0  ↓then  ↓go to L2
             ↓end ;  cr ;  ↓go to L1 ;
         L2:  cr ;
       ↓end
    ↓end ;
READREAL2(2,X,Y) ;  READARRAY6(6, f1a, f1b, f0a, f0b, f1, f0) ;
Output (7) ; cr ;
C:=1/X ;  D:=1/Y ;  K:=exp(-X) ;  L:=exp(-Y) ;
↓for  j:=0  ↓step 1  ↓until n  ↓do
↓for  j:=0  ↓step 1  ↓until n  ↓do
   ↓begin
      S1ba[i,-1]:=0 ;
      S1ba[i,j]:=(j×S1ba[i,j-1]+K×f1b[i]-f1[i+j])×C ;
      S0ba[i,-1]:=0 ;
      S0ba[i,j]:=(j×S1ba[i,j-1]+K×f0b[i]-f0[i+j])×C ;
      J:=i ;  I:=j ;
      S1ab[I,-1]:=0 ;
      S1ab[I, J]:=(J×S1ab[I,J-1]+f1a[I]-f1[I+J](×D ;
      S0ab[I,-1:=0 ;
      S0ab[I,J]:=(J×S0ab[I,J-1]+L×f0a(I)-f0[I+J])×D ;
      S1ab[I,n+1]:=S1ba[J,n+1]:=0 ;
      W0[I,J]:=S0ab[I,J]+S0ba[J,I] ;
   ↓end ;
↓for  j:=0  ↓Step 1  ↓until n  ↓do
↓for  i:=0  ↓step 1  ↓until n  ↓do
   W1[I,J]:=S1ab[I,J+1] ;
↓for  j:=0  ↓step 1  ↓until n-2  ↓do
↓for  i:=0  ↓step 1  ↓until n-2  ↓do
   ↓begin
      Z0[j,i]:=S0ab[j,i+2]+S0ab[i,j+2]+S1ab[j+1,i]S1ba[i×1,j]-2×W1
      [j+1,i+1] ;  W2[j,i]:=(W0[j,i]-3×Z0[j,i])/4 ;
   ↓end ;
↓for  j:=0  ↓step 1  ↓until n-3  ↓do
↓for  i:=0  ↓step 1  ↓until n-3  ↓do
```

```
          ↓begin
            Z1[j,i]:= 3 ※W 1 [j,i+ 2 ]+ 3 ※W 1 [j+ 2 ,i]-W 0 [j+ 1 ,i+ 1 ]-W 1 [j,i]- 5
            ※W 2 [j+ 1 ,i+ 1 ] ;
            W 3 [j,i]:= 4 ※W 1 [j,i]- 5 ※Z1[j,i])/ 9  ;
          ↓end
          PRINT('W 0 ',n,W 0 ) ;  PRINT(W 1 ,n,W 1 ) ;  PRINT('Z0',n- 2 ,Z0) ;
          PRINT('W 2 ,n- 2 ,W 2 ) ;  PRINT('Z1',n- 3 ,Z1) ;  PRINT('W 3 ',n- 3 ,W 3 );
          PRINT(S1ba,n,S1ba) ;  PRINT('S1aqn,S1ab) :
      ↓end
  ↓end ;
```

§ 4 謝　　　辞

本研究は東京大学物性研究所電子計算機室で FACOM—202— の電子計算機を使用した時の実際のプログラムである。

同計算機室長井上謙蔵氏，同室の高橋秀知氏，清水公子氏，中川雅子氏に大変に御世話になりこのプログラミングの大半はその指導によったものであることを記して，その御厚情を深く感謝する次第であります。

またこの機会を与えられた東大教授柿内賢信博士（東大物性研究所）には色々と御指導と御厚情を頂きまして深く感謝を捧げる次第であります。

この論文は著者が非常に御懇切な御指導と御鞭撻を頂きました恩師小谷正雄先生の還暦記念に捧げるものであります。