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APPENDIX A

FORTRAN IV PROGRAM FOR CALCULATING THE DENSITY OF STATES IN EYMARD AND DURAFFOURG METHOD

The variables used in the expressions for calculating the density of states are denoted by the folowing symbols in the FORTRAN IV program.

Varibles	Symbols in Program
MAIN PROGRAM	
ν(initial value)	PNU
ν(Final value)	PNUL
ξ'	CHI
π	PI
$a(\nu)$	A
$b(\nu)$	B
$\rho(E)$	DENSIT
REAL FUNCTION EMDU	
The variational expression	
Eq. (3.1.28)	EMDU

REAL FUNCTION DENS

$a(\nu)$	Eq.(3.1.25)	A
$b(\nu)$	Eq.(3.1.26)	B
$\rho(E)$	Eq.(3.1.27)	DENS

SUBROUTINE ROOT

The variational parameter x.	X

The other variables and some description see Ref. 37

MAIN PROGRAM

```
C       EMDU METHOD
        IMPLICIT REAL*8(A-H,O-Z)
        COMMON/GRO/PNU
        COMMON/GRI/CHI,PI
        COMMON/GR2/A,B,XR
        EXTERNAL EMDU
        ER=1.D-12
        PI=3.14159265358979323846 2DO
      1 READ(1,301)CHI,PNU,PNUL,DELN
        IF(DELN.EQ.O.DO) STOP
        WRITE(3,302) CHI
        N=1
        NOE=DLOG10(PNU)
        IF(PNU.LT.1.DO)NOE=NOE-1
        DELP=10.DO**NOE
        X=5.DO
      2 CONTINUE
        CALL ROOT (X,20.DO,1,1,EMDU,1.D-8,50.DO,MES,20,ER)
        IF(MES.NE.O)GO TO 3
        DENSIT=DENS(X)
        WRITE(3,303) PNU,X,A,B,DENSIT
        IF(N/5*5-N.EQ.O)WRITE(3,304)
        IF(N.NE.20) GO TO 4
        N=O
        WRITE(3,302) CHI
      4 N=N+1
      3 IF(DELP.GE.PNU*.999DO)DELP=DELP/10.DO
        PNU=PNU-DELN*DELP
        IF(DABS(PNU).LT.ER) PNU=DELP
        IF(PNU.GE.PNUL) GO TO 2
        GO TO 1
    301 FORMAT(4D20.15)
    302 FORMAT (1H1,'NUMERICAL RESULTS OF THE DENSITY OF STATES ANU B
       *R THE SCREENED COULOMB POTENTIAL'//20X,'CHI=    ',D14.6//4X,2H
       *X,1HX,24X,1HA,26X,1HB,27X, 3HRHO//1HO)
    303 FORMAT (1HO,D10.5,3X,4(D22.16,3X)
    304 FORMAT(1HO)
        END
        REAL FUNCTION EMDU*8(X)
        IMPLICIT REAL*8(A-H,O-Z)
        COMMON/GRO/PNU
        A=X*X*(1.DO+X*(12.DO+X*(68.DO+X*256.DO)))
        B=PNU*(3.DO+X*(36.DO+X*140.DO))
        EMDU=A-B
        RETURN
        END
```

```
      REAL FUNCTION DENS*8(X)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/GRO/PNU
      COMMON/GRI/CHI,PI
      COMMON/GR2/A,B,XR
      C=1.DO+X*10.DO
      D=1.DO+X*2.DO
      E=PNU+X*X
      F=(1.DO+X*(10.DO+X*32.DO))
      A=DSQRT((C**3)/F/3.DO)*((E/F*D/X)**3)*(D/PI)**2*(D**5)/1.5DO
      B=((E*D)**2)*(D/X)**3/F
      DENS=DEXP(-B/(2.DO*CHI))*A
      RETURN
      END
      SUBROUTINE ROOT (X,RANGE,M,L,FUN,BL,BU,MES,NOL,ERROR)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION V(100),XX(100),FF(100)
      IF(X.GT.BU.OR.X.LT.BL)GO TO 25
      B1=BL-ERROR
      B2-BU+ERROR
      IU=O
      IL=O
      MES=O
      XIN=X
      DEL=(BL-X)/RANGE
      IF(BU-X.LT.X-BL)DEL=(BU-X)/RANGE
    1 X2=X
      F2=FUN(X2)
      IF(F2.EQ.O.DO)RETURN
    2 X1=X2
      F1=F2
      X2=X2+DEL
      IF(X2.LT.81)GO TO 23
      IF(X2.GT.B2)GO TO 24
      F2=FUN(X2)
      IF(F2.EQ.O.DO)RETURN
      IF(L.EQ.O)GO TO 3
      SL=(F2-F1)/DEL*L
      IF(SL.LE.O.DO.AND.M.EQ.O)  GO TO2
      IF(SL.LE.O.DO)GO TO 4
    3 IF(F1/F2.LE.O.DO)GO TO 8
      IF(M.EQ.O)GO TO 2
      M=O
      IF(F1/F2.GT.1.DO)GO TO 2
```

```
 4 M=O
   IF(DEL.LT.O.)GO TO 6
   DEL=(BL-XIN)/RANGE
   GO TO 7
 6 DEL=(BU-XIN)/RANGE
 7 X2=X1
   F2=F1
   GO TO 2
 8 NG1=O
   NG2=O
 9 DO14N=1,5
   X=(X1*F2-X2*F1)/(F2-F1)
   F=FUN(X)
   IF(F.EQ.O.DO) RETURN
   XX(N)=X
   FF(N)=F
   IF(F/F1.LT.O.DO)GO TO 10
   F1=F
   X1=X
   NG1=1
   IF(NG2.EQ.O)F2=F2/2.DO
   IF(DABS(F2/F1).GT.20.)F2=-F1*20.
   GO TO 11
10 F2=F
   X2=X
   NG2=1
   IF(NG1.EQ.O)F1=F1/2.DO
   IF(DABS(F1/F2).GT.20.)F1=-F2*20.
11 IF(NG1.NE.NG2)GO TO 12
   NG1=0
   NG2=0
12 IF(N.LT.2)GO TO 14
   IJJ=N-1
   DO13J=1,IJJ
   IF(FF(N)/FF(J).LT.O.DO) GO TO 13
   IF(FF(N)/FF(J).GE.1.DO)GO TO 8
13 CONTINUE
   IF(DABS(F*(X2-X1)/(F2-F1)).LT.ERROR)GO TO 22
14 CONTINUE
   N=5
   KK=0
 5 DO 16J=2,N
16 V(J)=(XX(1)*FF(J)=XX(J)*FF(1))/(FF(J)-FF(1))
   X=V(N)
   IF(N.EQ.2.AND.KK.EQ.1) RETURN
   N1=N-1
```

```
      DO17K=2,N
      IJ=K+1
      DO17K=IJ,N
   17 V(J)=(V(K)*FF(J)-V(J)*FF(K))/(FF(J)-FF(K))
      X=V(N)
      IF(N.GE.NOL)MES=2
      IF(X.GT.BU.OR.X.LT.BL)MES=3
      IF(KK.EQ.1.OR.MES.NE.0)RETURN
      F=FUN(X)
      IF(F.EQ.0.DO)RETURN
      IF(F*F1.LT.0.DO) GO TO18
      F1=F
      X1=X
      GO TO 19
   18 F2=F
      X2=X
   19 N=N+1
      XX(N)=X
      FF(N)=F
      IJJ=N-1
      DO 20J=1,IJJ
      IF(FF(N)/FF(J).LT.0.DO) GO TO 20
      IF(FF(N)/FF(J).GE.1.DO)GO TO 8
   20 CONTINUE
      IF(DABS(F*(X-XX(N-1))/(F-FF(N-1))).LT. ERROR)KK=1
      GO TO 5
   22 KK=1
      GO TO 5
   23 IF(IU.EQ.1)GO TO 25
      X=XIN
      DEL=(BU-X)/RANGE
      IL=1
      GO TO 1
   24 IF(IL.EQ.1)GO TO 25
      X=XIN
      DEL=(BL-X)/RANGE
      IU=1
      GO TO 1
   25 MES=1
      RETURN
      ENS
```

APPENDIX B

FORTRAN IV PROGRAM FOR CALCULATING THE DENSITY OF STATES IN PRESENT METHOD

The variables used in the expressions for calculating the density of states are denoted by the following symbols in the FORTRAN IV program.

variables	Symbols in Program
MAIN PROGRAM	
ν(initial value)	PNU
ν(Final value)	PNUL
ξ'	CHI
π	PI
$a(\nu)$	A
$b(\nu)$	B
$\rho(E)$	DENSIT
REAL FUNCTION PCCU	
The variational expression Eq (3.2.58)	PCCU
REAL FUNCTION DENS	

REAL FUNCTION DENS

$a(\nu)$	Eq (3.2.56)	A
$b(\nu)$	Eq (3.2 57)	B
$\rho(E)$		DENS

SUBROUTINE ROOT

The variational parameter y	X

MAIN PROGRAM

```
C       PCCU METHOD
        IMPLICIT REAL*8(A-H,O-Z)
        COMMON/GRO/PNU
        COMMON/GRI/CHI,PI
        COMMON/GR2/A,B,XR
        EXTERNAL PCCU
        ER=1.D-12
        PI=3.1 4159265358979323846 2DO
      1 READ(1,301)CHI,PNU,PNUL,DELN
        IF(DELN.EQ.O.DO) STOP
        WRITE(3,302) CHI
        N=1
        NOE=DLOG10(PNU)
        IF(PNU.LT.1.DO)NOE=NOE-1
        DELP=10.DO**NOE
        X=5.DO
      2 CONTINUE
        CALL ROOT (X,20.DO,1,1,PCCU,1.D-8,50.DO,MES,20,ER)
        IF(MES.NE.0)GO TO 3
        DENSIT=DENS(X)
        WRITE(3,303) PNU,X,A,B,DENSIT
        IF(N/5*5-N.EQ.0)WRITE(3,304)
        IF(N.NE.20) GO TO 4
        N=0
        WRITE(3,302) CHI
      4 N=N+1
      3 IF(DELP.GE.PNU*.999DO)      DELP=DELP/10.DO
        PNU=PNU-DELN*DELP
        IF(DABS(PNU).LT.ER) PNU=DELP
        IF(PNU.GE.PNUL) GO TO 2
        GO TO 1
    301 FORMAT(4D20.15)
    302 FORMAT (1H1,'NUMERICAL RESULTS OF THE DENSITY OF STATES ANU BNU FO
       *R THE SCREENED COULOMB POTENTIAL'//20X,'CHI=   ',D14.6//4X,2HNU,18
       *X,1HX,24X,1HA,26X,1HB,27X, 3HRHO//1HO)
    303 FORMAT (1HO,D10.5,3X,4(D22.16,3X))
    304 FORMAT(1HO)
        END
```

```
      REAL FUNCTION PCCU*8(X)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/GRO/PNU
      A=X*X*(3.DO+X*(48.DO+X*(344.DO+X*(1472.DO+X*(3828.DO+X*9216.DO))))
     *)
      B=PNU*2.DO*(9.DO+X*(144.DO+X*(968.DO+X*(3392.DO+X*6604.DO))))
      PCCU=A-B
      RETURN
      END

      REAL FUNCTION DENS*8(X)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/GRO/PNU
      COMMON/GRI/CHI,PI
      COMMON/GR2/A,B,XR
      C=PNU*2.DO+X*X
      D=1.DO+X*2.DO
      E=(3.DO+X*(42.DO+X*(244.DO+X*(728.DO+X*1152.DO))))
      F=(1.DO+X*(14.DO+X*(60.DO+X*264.DO)))
      A=DSQRT((F/27.DO)**3/E)*((C*D/X/E)**3)*(D/PI)**2*(D**9)*546.DO
      B=((C*D)**2)*(D/X)**3*(D**2)*9.DO/(4.DO*E)
      DENS=DEXP(-B/(2.DO*CHI))*A
      RETURN
      END
```

APPENDIX C

FORTRAN IV PROGRAM FOR CALCULATING THE DENSITY OF STATES FOR THE CASE OF GAUSSIAN IMPURITY POTENTIAL IN PRESENT METHOD

The variable used in the expressions for calculating the density of states are denoted by the following symbols in the FORTRAN IV program.

variables	Symbols in Program
MAIN PROGRAM	
ν(initial value)	PNU
ν(Final value) n	PNUL
ξ'	CHI
The variational parameter Z	X
n(ν) Eq (3.2. 29)	GN
a(ν) Eq (3.2. 27)	A
b(ν) Eq.(3.2. 28)	B
ρ(E) Eq (3.2. 22)	DENSIT

MAIN PROGRAM

```
C      GAUSSIAN POTENTIAL
       IMPLICIT REAL *8(A-H,O-Z)
       ER=1.D-12
       PI=3.14159265358979323846 2DO
     1 READ(1,301)  CHI,PNU,PNUL,DELN
       IF(DELN.EQ.O.DO) STOP
       WRITE(3,302) CHI
       N=1
       NOE=DLOG10(PNU)
       IF(PNU.LT.1.DO) NOE=NOE-1
       DELP=10.DO**NOE
     2 C=1.DO+16.DO*PNU
       D=DSQRT(O)
       X=(D-1.DO)/2.DO
       GN=32.DO*PNU/((D-1.DO)*(D+7.DO))
       A=DSQRT((D-1.DO)**3)*DSQRT((D+7.DO)**9)/DSQRT(2.DO**25)PI**2
       B=DSQRT(D-1.DO)*DSQRT((D+7.DO)**7)/2.DO**8
       DENSIT=DEXP(-B/(2.DO*CHI))*A
       WRITE(2,303)PNU,X,GN,A,B,DENSIT
       IF(N/5*5-N.EQ.O) WRITE(2,304)
       IF(N.NE.25) GO TO 3
       N=O
       WRITE(3,302) CHI
     2 N=N+1
       IF(DELP.GE.PNU*.999DO)DELP=DELP/10.DO
       PNU=PNU-DELN*DELP
       IF( DABS(PNU).LT.ER)PNU=DELP
       IF(PNU.GE.PNUL) GO TO 2
       GO TO 1
   301 FORMAT(4D20.15)
   302 FORMAT(1H1,'NUMERICAL RESULTS FOR THE GAUSSIAN POTENTIAL'//20X,'CH
      *I=',D14.6//4X,2HNU,18X,1HX,24X,1HN,22X,1HA,24X,1HB,23X,3HRHO/1HO)
   303 FORMAT(1HO,D10.4,2X,5(D22.16,2X))
   304 FORMAT(1HO)
       END
```

VITA

My name is Pachernchai Chaiyasith. I was born in Ubonratchathani on August 20, 1957. I was awarded a B.Ed. degree in Chemistry from Srinakharinwirot University (Prasarnmitr Campus) in 1979. I was supported by the University Development Commission Scholarship during the study towards the Master's degree of Science. After my graduation I shall be an instructor at the Department of Applied Chemistry, King Mongkut's Institute of Technology (Chao Khuntahan Lat Krabang Campus).