OpenMX 朗読会

“The Journey in OpenMX” ver.1.0

Let’s trace the calculation process in OpenMX !!

・Review of equations used in OpenMX

・Decoding of subroutines step by step

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Kohn-Sham equaton: $\left[-\frac{\hbar^2\nabla^2}{2m}+\tilde{V}_{\text{eff}}\left(\mathbf{r}\right)\right]\psi_k\left(\mathbf{r}\right)=\varepsilon_k\psi_k\left(\mathbf{r}\right)$

$$\begin{aligned}\tilde{V}_{\text{eff}}\left(\mathbf{r}\right)&=\tilde{V}_{\text{core}}\left(\mathbf{r}\right)+\tilde{V}_{\text{Hartree}}\left(\mathbf{r},\mathbf{r}'\right)+\tilde{V}_{\text{xc}}\left(\mathbf{r}\right)\\&=\tilde{V}_{\text{nonlocal}}\left(\mathbf{r}\right)+\tilde{V}_{\text{na}}\left(\mathbf{r}\right)+\tilde{V}_{\delta\text{Hartree}}\left(\mathbf{r},\mathbf{r}'\right)+\tilde{V}_{\text{xc}}\left(\mathbf{r}\right)\end{aligned}$$ in OpenMX

$\psi_k\left(\mathbf{r}\right)=\sum_{i=1}^{N_{\text{PAO}}}C_{ki}\phi_i\left(\mathbf{r}\right)$: linear expansion of wave functions with basis set (PAO)

$$\mathbf{HC}_k=\varepsilon_k\mathbf{SC}_k \qquad \mathbf{C}_k=\begin{pmatrix}C_{k1}\\ \vdots\\ C_{kN_{\text{PAO}}}\end{pmatrix}$$

Kohn-Sham equation ⇒ Generalized eienvalue problem

The bundle of coefficients and eigenvalue can be expressed in a matrix form:

$$\mathbf{C}_k = \begin{pmatrix} C_{k1} \\ \vdots \\ C_{kN_{\mathrm{PAO}}} \end{pmatrix} \quad \Rightarrow \quad \mathbf{C} = \begin{pmatrix} C_{11} & \cdots & C_{1N_{\mathrm{PAO}}} \\ \vdots & \ddots & \vdots \\ C_{N_{\mathrm{PAO}}1} & \cdots & C_{N_{\mathrm{PAO}}N_{\mathrm{PAO}}} \end{pmatrix}$$

$$\varepsilon_k \quad \Rightarrow \quad \boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \varepsilon_{N_{\mathrm{PAO}}} \end{pmatrix}$$

In this case, $\mathbf{HC}_k = \varepsilon_k \mathbf{SC}_k \quad \Rightarrow \quad \mathbf{HC} = \boldsymbol{\varepsilon}\mathbf{SC}$

Matrix elements in equation “**HC = εSC**”

$$S_{ij} = \int \phi_i(\mathbf{r})\phi_j(\mathbf{r})d\mathbf{r}$$ Overlap matrix

$$H_{ij} = T_{ij} + V_{ij}^{\mathrm{na}} + V_{ij}^{\delta\mathrm{H}} + V_{ij}^{\mathrm{xc}} + V_{ij}^{\mathrm{nl}}$$ Hamiltonian matrix

$$T_{ij} = \int \phi_i(\mathbf{r})\frac{-\hbar^2\nabla^2}{2m}\phi_j(\mathbf{r})d\mathbf{r}$$ Kinetic matrix

$$V_{ij}^{\delta\mathrm{H}} = \int \phi_i(\mathbf{r})\tilde{V}_{\delta\mathrm{Hartree}}(\mathbf{r})\phi_j(\mathbf{r})d\mathbf{r}$$

$$= \iint \phi_i(\mathbf{r})\frac{\delta\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\phi_j(\mathbf{r})d\mathbf{r}'d\mathbf{r}$$ Difference Hartree potential matrix

$$V_{ij}^{\mathrm{na}} = \int \phi_i(\mathbf{r})\tilde{V}_{\mathrm{na}}(\mathbf{r})\phi_j(\mathbf{r})d\mathbf{r}$$ Neutral atomic potential matrix

$$V_{ij}^{\mathrm{xc}} = \int \phi_i(\mathbf{r})\tilde{V}_{\mathrm{xc}}(\mathbf{r})\phi_j(\mathbf{r})d\mathbf{r}$$ Exchange-correlation potential matrix

$$V_{ij}^{\mathrm{nl}} = \int \phi_i(\mathbf{r})\tilde{V}_{\mathrm{nonloacl}}(\mathbf{r})\phi_j(\mathbf{r})d\mathbf{r}$$ Nonlocal potential matrix

Main process of calculation in OpenMX

STEP 1: Preparation of basis sets and pseudopotentials

STEP 2: Set of real-space grids

STEP 3: Calculation of matrix elements

STEP 4: Solving generalized eigenvalue problem

STEP 5: SCF calculation（convergence problem）

STEP 6: Force calculation

STEP 7: Calculation of physical quantities

OpenMX

Program	Function	corresponding STEP
openmx.c	Main program	
readfile.c	Reading files	
Input_std.c	Reading input file for atomic structure and calculation conditions	
SetPara_DFT.c	Reading database for basis sets and pseudopotentials	
ReadPara_DFT		1
Read_PAO	Reading basis sets (PAO)	1
Read_VPS	Reading pseudopotentials (VPS)	1
V_Hart_atom	Calculation of atomic Hartree potentials	1
Vna	Calculation of neutral atomic potentials	1
FT_PAO	Fourier transformation of PAOs	1
FT_NLP	Fourier transformation of non-local parts	1
truncation.c	Preparation of real-space grids Storage of relationship between real-space grids and parameters	2
DFT.c	SCF calculation of electronic structure	3，4，5

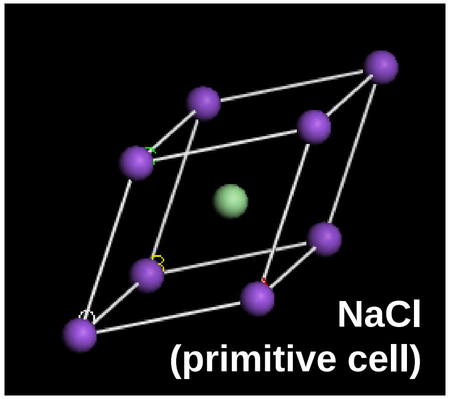
DFT.c (in case of solver = “Cluster”)

SCF calculation			DFT.c	
Hamiltonian matrix (H) elements			Set_OLP_Kin.c	Overlap integrals, kinetic-energy terms
			Set_Nonlocal.c	Non-local terms
			Set_ProExpn_VNA.c	Projector expansion method
SCF	Const. of H	iter. = 1	Set_Aden_Grid.c	Superposition of elec. densities of isolated atoms
			Set_Orbital_Grid.c	Set
			FFT_Density.c	Fourier transformation of electronic densities
			Poisson.c	Hartree potential
			Set_Hamiltonian.c	Hamiltonian matrix
			Set_Vpot.c	neutral atomic, xc, and Hartree potentials
		iter. ≥ 2	Poisson.c	δ–Hartree potentials
			Set_Hamiltonian.c	Hamiltonian matrix
			Set_Vpot.c	neutral atomic, xc, and δ–Hartree potentials
	Generalized eigenvalue problem		Cluster_DFT.c※	HC = εSC (※ in case of solver = “Band”, the subroutine is “Band_DFT_Col.c”)
	Physical quantities		Mulliken_Charge.c Band_DFT_kpath.c, etc.	Mulliken charge Band structure, etc...
	Conv. algorithm	every iter.	(check SCF-convergence)	
		In case of no conv.	Mixing_DM.c	Mixing of previous and present density matrices (DM)
			Set_Density_Grid.c	Calculation of charge-density grid from DM

Preparation of Band Calculation

"NaCl.dat"

```
Atoms.Number              2
Atoms.SpeciesAndCoordinates.Unit    Ang # Ang|AU
<Atoms.SpeciesAndCoordinates            # Unit=Ang.
  1   Na   0.00000  0.00000  0.00000    4.5 4.5
  2   Cl   2.81500  2.81500  2.81500    3.5 3.5
Atoms.SpeciesAndCoordinates>
Atoms.UnitVectors.Unit              Ang #  Ang|AU
<Atoms.UnitVectors                      # unit=Ang.
  0.00000   2.81500   2.81500
  2.81500   0.00000   2.81500
  2.81500   2.81500   0.00000
Atoms.UnitVectors>


#
# SCF or Electronic System
#

scf.XcType                 LDA         # LDA|LSDA-CA|LSDA-PW
scf.SpinPolarization       off         # On|Off
scf.ElectronicTemperature  300.0       # default=300 (K)
scf.energycutoff           150.0       # default=150 (Ry)
scf.maxIter                170         # default=40
scf.EigenvalueSolver       band        # Recursion|Cluster|Band
scf.Kgrid                  3 3 3       # means 4x4x4
scf.Mixing.Type           rmm-diisk    # Simple|Rmm-Diis|Gr-Pulay
scf.Init.Mixing.Weight     0.010       # default=0.30
scf.Min.Mixing.Weight      0.001       # default=0.001
scf.Max.Mixing.Weight      0.200       # default=0.40
scf.Mixing.History          6          # default=5
scf.Mixing.StartPulay      12          # default=6
scf.criterion             1.0e-6       # default=1.0e-6 (Hartree)
scf.system.charge          0.0         # default=0.0
```



a : (**tv**[1][1], **tv**[1][2], **tv**[1][3])
b : (**tv**[2][1], **tv**[2][2], **tv**[2][3])
c : (**tv**[3][1], **tv**[3][2], **tv**[3][3])

Solver = 3

Kspace_grid1 = 3
Kspace_grid2 = 3
Kspace_grid3 = 3

🟨 … in "Input_std.c"

Outline of Subroutine “Band_DFT_Col.c”

1. Setting $\mathbf{k}$-mesh points

2. Searching first-neighbor atoms (determination of $\mathbf{R}_n$-region)

3. Setting overlap and Hamiltonian matrices for 3-D periodic boundary condition

4. Solving generalized eigenvalue problem

5. Finding chemical potential

6. Constructing density matrix (⇒ Check of SCF-convergence)

K-points (1); Weight Factor for DOS

Kspace_grid1
Kspace_grid2
Kspace_grid3

$\Rightarrow$

knum_i
knum_j
knum_k

in “Band_DFT_Col.c”

```
 for (i=0;i<=knum_i-1;i++) {
      for (j=0;j<=knum_j-1;j++) {
        for (k=0;k<=knum_k-1;k++) {
          k_op[i][j][k]=-999;
        }
      }
   }

   for (i=0;i<=knum_i-1;i++) {
     for (j=0;j<=knum_j-1;j++) {
       for (k=0;k<=knum_k-1;k++) {
         if ( k_op[i][j][k]==-999 ) {
           k_inversion(i,j,k,knum_i,knum_j,knum_k,&ii,&ij,&ik);
           if ( i==ii && j==ij && k==ik ) {
             k_op[i][j][k]     = 1;
           }

           else {
             k_op[i][j][k]     = 2;
             k_op[ii][ij][ik]  = 0;
           }
         }
       } /* k */
     } /* j */
   } /* i */
```

i	0	1	2
ii	2	1	0

inversion

k_op[i][j][k] : weight factor

***l*. 426 in “Band_DFT_Col.c”**

K-points (2); Weight Factor for DOS

ex) case of 2-dimensional k-space (3 × 3)

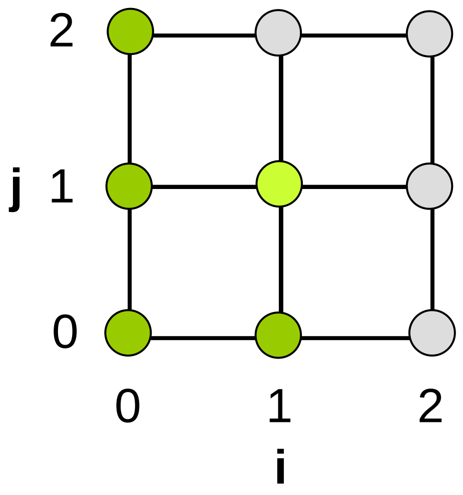
loop	(i,j)			(ii,ij)	
1	0	0		2	2
2	0	1		2	1
3	0	2		2	0
4	1	0		1	2
5	1	1		1	1
6	1	2			
7	2	0			
8	2	1			
9	2	2			

k_op = 2

k_op = 0

k_op = 1
(Γ point)

skipped
because **k_op**[i][j] ≠ –999



K-points (3); K-Grids by Regular Mesh

from *l*. 467 in "Band_DFT_Col.c"

```
/* set T_KGrids1,2,3 and T_k_op */

   T_knum = 0;
   for (i=0; i<knum_i; i++){

     if (knum_i==1)  k1 = 0.0;
     else            k1 = -0.5 + (2.0*(double)i+1.0)/(2.0*(double)knum_i)
                          + Shift_K_Point;

     for (j=0; j<knum_j; j++){

       if (knum_j==1)  k2 = 0.0;
       else            k2 = -0.5 + (2.0*(double)j+1.0)/(2.0*(double)knum_j)
                            - Shift_K_Point;

       for (k=0; k<knum_k; k++){

         if (knum_k==1)  k3 = 0.0;
         else            k3 = -0.5 + (2.0*(double)k+1.0)/(2.0*(double)knum_k)
                              + 2.0*Shift_K_Point;

         if (0<k_op[i][j][k]){

           T_KGrids1[T_knum] = k1;
           T_KGrids2[T_knum] = k2;
           T_KGrids3[T_knum] = k3;
           T_k_op[T_knum]    = k_op[i][j][k];

           T_knum++;
         }
       }
     }
   }
```

K-grids with non-zero weight (1-D array)

1-dimensionalization of **k_op**[i][j][k]

(After loop processing) total num. of k-points with non-zero weight

Before K-Loop; 1-Dimensionalizing S and H Matrices

```
 /* set S1 */

if (SCF_iter==1 || all_knum!=1){
   size_H1 = Get_OneD_HS_Col(1, CntOLP,   S1, MP, order_GA, My_NZeros, SP_NZeros, SP_Atoms);
 }

diagonalize1:

  /* set H1 */

  if (SpinP_switch==0){
    size_H1 = Get_OneD_HS_Col(1, nh[0], H1,   MP, order_GA, My_NZeros, SP_NZeros, SP_Atoms);
  }
  else if (1<numprocs0){
    size_H1 = Get_OneD_HS_Col(1, nh[0], H1,   MP, order_GA, My_NZeros, SP_NZeros, SP_Atoms);
    size_H1 = Get_OneD_HS_Col(1, nh[1], CDM1, MP, order_GA, My_NZeros, SP_NZeros, SP_Atoms);

    if (myworld1){
      for (i=0; i<size_H1; i++){
        H1[i] = CDM1[i];
      }
    }
  }
  else{
    size_H1 = Get_OneD_HS_Col(1, nh[spin], H1, MP, order_GA, My_NZeros, SP_NZeros, SP_Atoms);
  }
```

because S do not change until the next MD-step starts

Overlap matrix : **CntOLP** (= **OLP** in DFT.c) ⇒ **S1**

Hamiltonian matrix : **nh** (= **H** in DFT.c) ⇒ **H1**

Starting point in 1-D array of each atom

from *l*. 773 in "Band_DFT_Col.c"

In case of basis sets, "Na9.0-s1p1" and "Cl7.0-s1p1"...

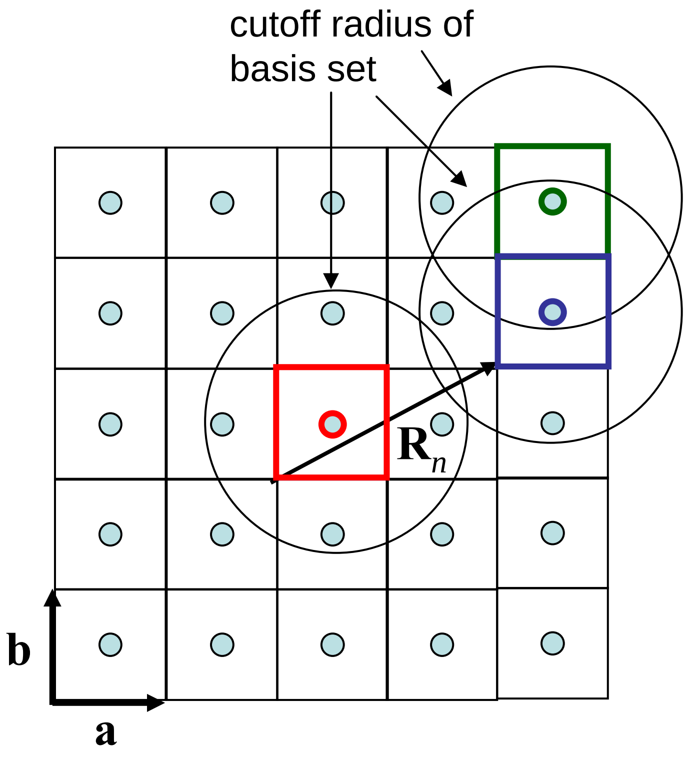
atom	1 (Na)				2 (Cl)			
PAO	1 (s)	2 (p_x)	3 (p_y)	4 (p_z)	1 (s)	2 (p_x)	3 (p_y)	4 (p_z)
1-D index	1	2	3	4	5	6	7	8
MP[atom]	1				5			

K-Loop (1); S and H for 3-D Periodic Boundary Condition

$$S_{ij}(\mathbf{k}) = \sum_{\mathbf{R}_n} e^{i\mathbf{k}\cdot\mathbf{R}_n} \underbrace{\int \phi_i(\mathbf{r})\phi_j(\mathbf{r}-\mathbf{R}_n)\,d\mathbf{r}}_{\textbf{OLP}\text{ (in DFT.c)}}$$

$$H_{ij}(\mathbf{k}) = \sum_{\mathbf{R}_n} e^{i\mathbf{k}\cdot\mathbf{R}_n} \underbrace{\int \phi_i(\mathbf{r})\bar{H}\phi_j(\mathbf{r}-\mathbf{R}_n)\,d\mathbf{r}}_{\textbf{H}\text{ (in DFT.c)}}$$

- $\mathbf{R}_n = k\mathbf{a} + l\mathbf{b} + m\mathbf{c}$
- $\mathbf{R}_n$'s are determined as first-neighbor atoms in 3-D periodic boundary system.
- $\mathbf{R}_n$ is corresponding to each first-neighbor atom.



ex) a simple case: one atom per cell

○ is a first-neighbor atom of ○
○ is not a first-neighbor atom of ○

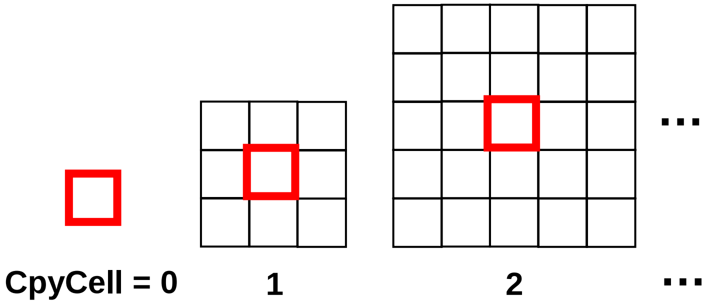
K-Loop (2); vector $\mathbf{R}_n$ (= $k\mathbf{a} + l\mathbf{b} + m\mathbf{c}$)

from *l.* 216 in "truncation.c"

```
CpyCell = 0;
   po = 0; TFNAN = 0; TSNAN = 0;

   do{

     CpyCell++;

     /***********************************************
          allocation of arrays listed above and
                Generation_ATV(CpyN);
     ***********************************************/

     TCpyCell = Set_Periodic(CpyCell,0);

     /***********************************************
       find Max_FSNAN by the physical truncation
         for allocation of natn, ncn, and Dis
     ***********************************************/

     Estimate_Trn_System(CpyCell,TCpyCell,0);

     /***********************************************
             allocation of natn, ncn, and Dis
     ***********************************************/

     Allocate_Arrays(3);
```

while po = 0 (see the next page)

generation of **atv**'s (= $\mathbf{R}_n$)



$$\left\{\begin{aligned} k\mathbf{a} &= \textbf{atv}[n][1] \\ l\mathbf{b} &= \textbf{atv}[n][2] \\ m\mathbf{c} &= \textbf{atv}[n][3] \end{aligned}\right.$$

$$\left\{\begin{aligned} k &= \textbf{atv\_ijk}[n][1] \\ l &= \textbf{atv\_ijk}[n][2] \\ m &= \textbf{atv\_ijk}[n][3] \end{aligned}\right.$$

```
    /**********************
     find TFNAN and TSNAN
    **********************/

    TFNAN2 = TFNAN;
    TSNAN2 = TSNAN;

   Trn_System(MD_iter,CpyCell,TCpyCell,0,1);

    if ( TFNAN==TFNAN2 && TSNAN==TSNAN2 && (Solver==1 || Solver==5
                                         || Solver==6 || Solver==8) ) po++;
    else if (TFNAN==TFNAN2 && (Solver==2 || Solver==3 || Solver==4
                                         || Solver==7 || Solver==9) ) po++;
    else if (CellNN_flag==1)                                          po++;

    Free_truncation(CpyCell,TCpyCell,0);

 } while (po==0);
```

- the index of $\mathbf{R}n$ between GAth and LBth atoms "**ncn**[GA][LB]"
- the number of first-neighbor atoms of *m*th atom "**FNAN**[m]"

- By increasing "CpyCell", one can search some point where the num. of first-neighbor atoms does not change moreover

⇒ finding range of $\mathbf{R}_n$

K-Loop (3); S and H matrices

from *l*. 809 in "Band_DFT_Col.c"

```
for (kloop0=0; kloop0<num_kloop0; kloop0++){

   kloop = S_knum + kloop0;

   k1 = T_KGrids1[kloop];
   k2 = T_KGrids2[kloop];
   k3 = T_KGrids3[kloop];

k = 0;
   for (AN=1; AN<=atomnum; AN++){
     GA_AN = order_GA[AN];
     wanA = WhatSpecies[GA_AN];
     tnoA = Spe_Total_CNO[wanA];
     Anum = MP[GA_AN];

     for (LB_AN=0; LB_AN<=FNAN[GA_AN]; LB_AN++){
       GB_AN = natn[GA_AN][LB_AN];
       Rn = ncn[GA_AN][LB_AN];
       wanB = WhatSpecies[GB_AN];
       tnoB = Spe_Total_CNO[wanB];
       Bnum = MP[GB_AN];

       l1 = atv_ijk[Rn][1];
       l2 = atv_ijk[Rn][2];
       l3 = atv_ijk[Rn][3];
       kRn = k1*(double)l1 + k2*(double)l2 + k3*(double)l3;

       si = sin(2.0*PI*kRn);
       co = cos(2.0*PI*kRn);
```

$$\mathbf{k} = 2\pi\frac{\mathbf{b}\times\mathbf{c}}{\Delta V}k_1 + 2\pi\frac{\mathbf{c}\times\mathbf{a}}{\Delta V}k_2 + 2\pi\frac{\mathbf{a}\times\mathbf{b}}{\Delta V}k_3$$

$$\left(\Delta V = \mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})\right)$$

$$\mathbf{R}_n = k\mathbf{a} + l\mathbf{b} + m\mathbf{c}$$

$$\therefore \mathbf{k}\cdot\mathbf{R}_n = 2\pi\left(k_1 k + k_2 l + k_3 m\right)$$

$$\sum_{\mathbf{R}_n} \boxed{e^{i\mathbf{k}\cdot\mathbf{R}_n}} \int d\mathbf{r}\cdots$$

```
        for (i=0; i<tnoA; i++){

          for (j=0; j<tnoB; j++){

            H[Anum+i][Bnum+j].r += H1[k]*co;
            H[Anum+i][Bnum+j].i += H1[k]*si;

            k++;

          }


          if (SCF_iter==1 || all_knum!=1){

            k -= tnoB;

            for (j=0; j<tnoB; j++){

              S[Anum+i][Bnum+j].r += S1[k]*co;
              S[Anum+i][Bnum+j].i += S1[k]*si;

              k++;
            }
          }

        }
      }
    }
```

$$H_{ij}(\mathbf{k}) = \boxed{\sum_{\mathbf{R}_n}} e^{i\mathbf{k}\cdot\mathbf{R}_n} \int \phi_i(\mathbf{r}) \bar{H} \phi_j(\mathbf{r}-\mathbf{R}_n) d\mathbf{r}$$

$$S_{ij}(\mathbf{k}) = \boxed{\sum_{\mathbf{R}_n}} e^{i\mathbf{k}\cdot\mathbf{R}_n} \int \phi_i(\mathbf{r}) \phi_j(\mathbf{r}-\mathbf{R}_n) d\mathbf{r}$$

K-Loop (4); Solving Eigenvalue Problem (Outline)

[1] $$\mathbf{HC} = \boldsymbol{\varepsilon}\mathbf{SC}$$: generalized eigenvalue problem

[2] $$\mathbf{U}^{\dagger}\mathbf{SU} = \mathbf{s}$$: diagonalization of $\mathbf{S}$ (solving eigenvalue problem for $\mathbf{S}$)

[3] $$\begin{cases} \mathbf{X} = \mathbf{U}\mathbf{s}^{-1/2} \\ \mathbf{X}^{\dagger} = \left(\mathbf{s}^{-1/2}\right)^{\dagger}\mathbf{U}^{\dagger} \\ \left(\mathbf{X}^{\dagger}\mathbf{SX} = \mathbf{I}\right) \end{cases}$$: canonical orthogonalization of $\mathbf{S}$

[4] $$\mathbf{X}^{\dagger}\mathbf{HXX}^{\dagger}\mathbf{C} = \boldsymbol{\varepsilon}\mathbf{X}^{\dagger}\mathbf{SXX}^{\dagger}\mathbf{C}$$: introducing $\mathbf{X}$ into $\mathbf{HC} = \boldsymbol{\varepsilon}\mathbf{SC}$

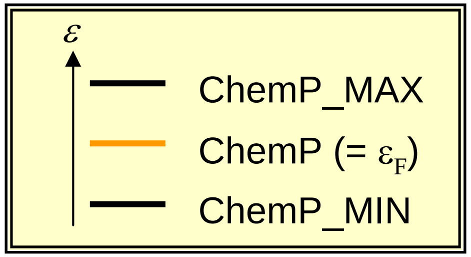
[5] $$\mathbf{H}'\mathbf{C}' = \boldsymbol{\varepsilon}\mathbf{C}'$$: standard eigenvalue problem

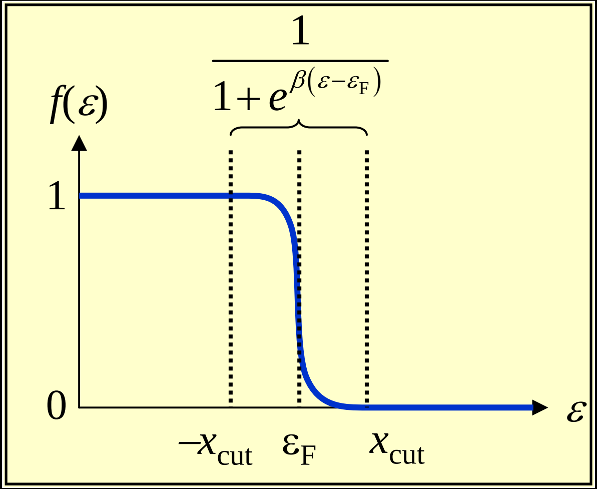
The detail can be checked in the supplemental documentation "*Eigenvalue_Problem_(in_Band_DFT_Col.c)*".

K-Loop (5); Finding Chemical Potential

```
  po = 0;
  loop_num = 0;
  ChemP_MAX = 10.0;
  ChemP_MIN =-10.0;

  do {

    loop_num++;

    ChemP = 0.50*(ChemP_MAX + ChemP_MIN);
    Num_State = 0.0;

    for (kloop=0; kloop<T_knum; kloop++){
      for (spin=0; spin<=SpinP_switch; spin++){
        for (l=1; l<=MaxN; l++){

          x = (EIGEN[spin][kloop][l] - ChemP)*Beta;

          if (x<=-x_cut)        FermiF = 1.0;
          else if (x>=x_cut)    FermiF = 0.0;
          else                  FermiF = 1.0/(1.0 + exp(x));

          Num_State += FermiF*(double)T_k_op[kloop];
        }
      }
    }

    if (SpinP_switch==0)
      Num_State = 2.0*Num_State/sum_weights;
    else
      Num_State = Num_State/sum_weights;

    Dnum = TZ - Num_State - system_charge;

    if (0.0<=Dnum)  ChemP_MIN = ChemP;
    else            ChemP_MAX = ChemP;
    if (fabs(Dnum)<10e-14)  po = 1;
  }
  while (po==0 && loop_num<2000);
```

from *l*.1462 in "Band_DFT_Col.c"





Num_state = $f(\varepsilon)w(\mathbf{k})\sum_{\mathbf{k},l} n_{\mathbf{k},l}$

$w(\mathbf{k})$: T_k_op

$n_{\mathbf{k},l}$: occupancy (= 0 or 1)

TZ : total valence charge

- Dnum > 0 : running short of electrons

  ⇒ put Fermi level upper
- Dnum < 0 : having excess electrons

  ⇒ put Fermi level lower

K-Loop (6); Density Matrix $\rho_{ij}(\mathbf{R}_n)$

$$\rho_{ij}\left(\mathbf{R}_n\right)=\frac{1}{V_{\mathrm{B}}}\int_{\mathrm{B}}d\mathbf{k}\sum_{l}^{\mathrm{occ.}}\mathrm{e}^{i\mathbf{R}_n\cdot\mathbf{k}}c_{l,i}^{*}\left(\mathbf{k}\right)c_{l,j}\left(\mathbf{k}\right)$$

from *l*. 2498 in "Band_DFT_Col.c"

```
for (AN=1+OMPID; AN<=atomnum; AN+=Nthrds){

        GA_AN = order_GA[AN];
        wanA = WhatSpecies[GA_AN];
        tnoA = Spe_Total_CNO[wanA];
        Anum = MP[GA_AN];

        k = (int)H[0][AN].r;

        for (LB_AN=0; LB_AN<=FNAN[GA_AN]; LB_AN++){
          GB_AN = natn[GA_AN][LB_AN];
          Rn = ncn[GA_AN][LB_AN];
          wanB = WhatSpecies[GB_AN];
          tnoB = Spe_Total_CNO[wanB];
          Bnum = MP[GB_AN];

          l1 = atv_ijk[Rn][1];
          l2 = atv_ijk[Rn][2];
          l3 = atv_ijk[Rn][3];
          kRn = k1*(double)l1 + k2*(double)l2 + k3*(double)l3;

          si = sin(2.0*PI*kRn);
          co = cos(2.0*PI*kRn);
```

$$\mathbf{k}=2\pi\frac{\mathbf{b}\times\mathbf{c}}{\Delta V}k_1+2\pi\frac{\mathbf{c}\times\mathbf{a}}{\Delta V}k_2+2\pi\frac{\mathbf{a}\times\mathbf{b}}{\Delta V}k_3$$

$$\left(\Delta V=\mathbf{a}\cdot\left(\mathbf{b}\times\mathbf{c}\right)\right)$$

$$\mathbf{R}_n=k\mathbf{a}+l\mathbf{b}+m\mathbf{c}$$

$$\therefore\mathbf{k}\cdot\mathbf{R}_n=2\pi\left(k_1k+k_2l+k_3m\right)$$

$$e^{i\mathbf{k}\cdot\mathbf{R}_n}$$

```
        for (i=0; i<tnoA; i++){

               ia = Anum + i;

               for (j=0; j<tnoB; j++){

                 jb = Bnum + j;

          d1 = 0.0;
          d2 = 0.0;

          for (l=1; l<=lmax; l++){

           tmp = co*(H[ia][l].r*H[jb][l].r + H[ia][l].i*H[jb][l].i)
                -si*(H[ia][l].r*H[jb][l].i - H[ia][l].i*H[jb][l].r);

            d1 += VecFkw[l]*tmp;
            d2 += VecFkwE[l]*tmp;;

          }

          CDM1[k] += d1;
          EDM1[k] += d2;

          /* increment of k */

          k++;

        }
      }
    }
  }
```

Summation and integration with regard to **k** and *l*

$$\sum_{l}^{\text{occ.}} \int d\mathbf{k} \cdots$$

summation of conjugated terms

$$e^{i\mathbf{R}_n\cdot\mathbf{k}} c_{l,i}^{*}(\mathbf{k}) c_{l,j}(\mathbf{k}) + e^{-i\mathbf{R}_n\cdot\mathbf{k}} c_{l,i}(\mathbf{k}) c_{l,j}^{*}(\mathbf{k})$$

1-D index for (i, j) and $\mathbf{R}_n$

Density matrix is used in checking SCF-converge