Structure of OPENMX extension: NEGF

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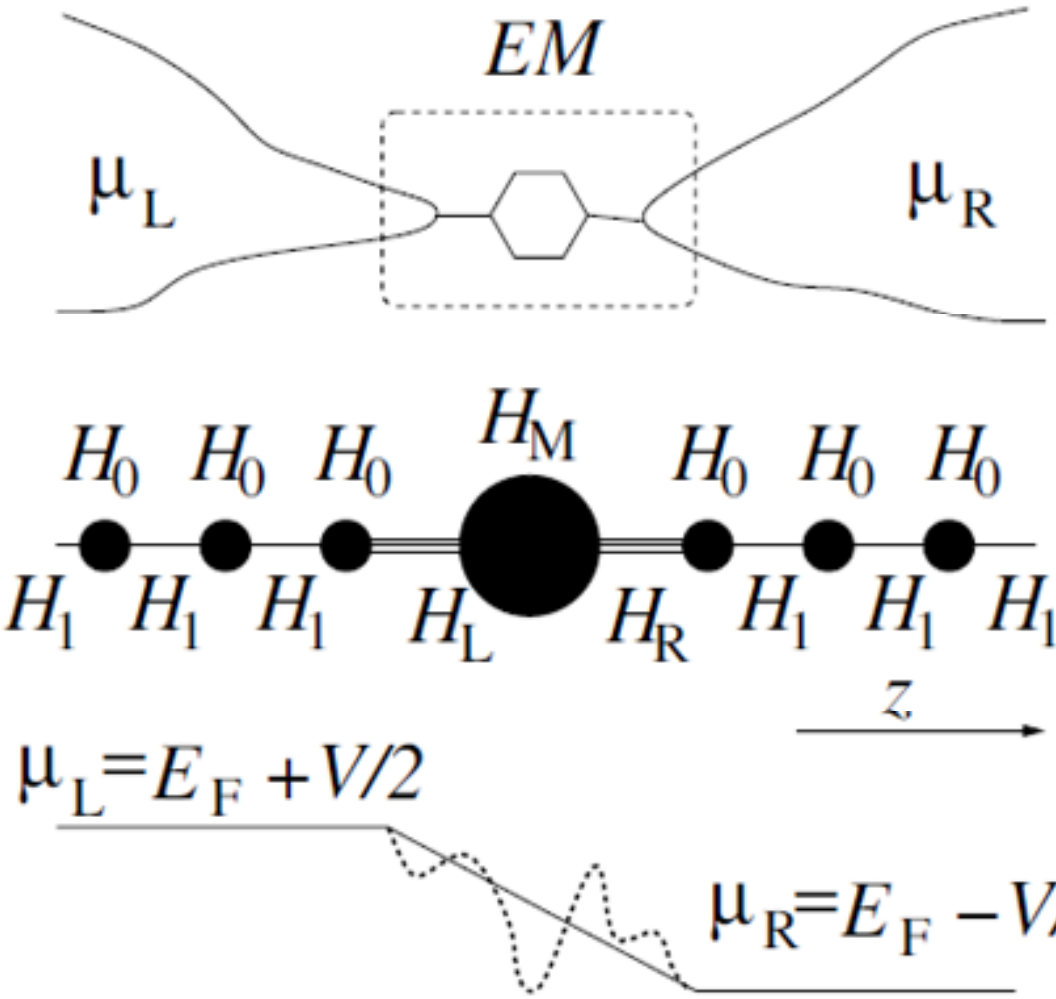
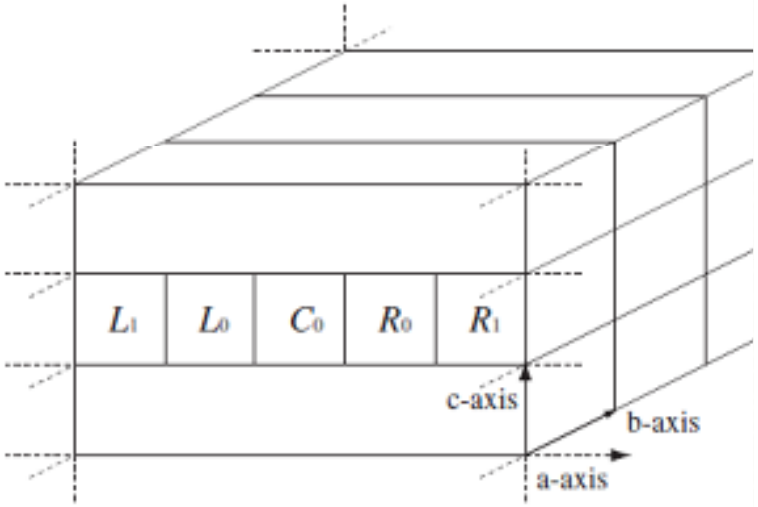
The configuration under consideration



(1)L,C,R regions

(2)C is extended.



The transport algorithm in OPENMX

Lead's self-energies

$$\Sigma_L = \left(ES_{CL} - H_{CL}\right) g_L \left(ES_{LC} - H_{LC}\right)$$

$$\Gamma_L = i\left[\Sigma_L - \Sigma_L^+\right]$$

$g_L =$ **surface Green function**

Kohn-Sham Hamiltonian

$$\hat{H}[n]\psi_i = \left[\hat{T} + V_{eff}\right]\psi_i = \varepsilon_i \psi_i$$

Scatter's Green's function

$$G^R = \left[ES - H[n] - \Sigma_L - \Sigma_R\right]^{-1}$$

Non-equilibrium density matrix

$$\rho^{neq} = \rho^{eq} + \Delta\rho$$

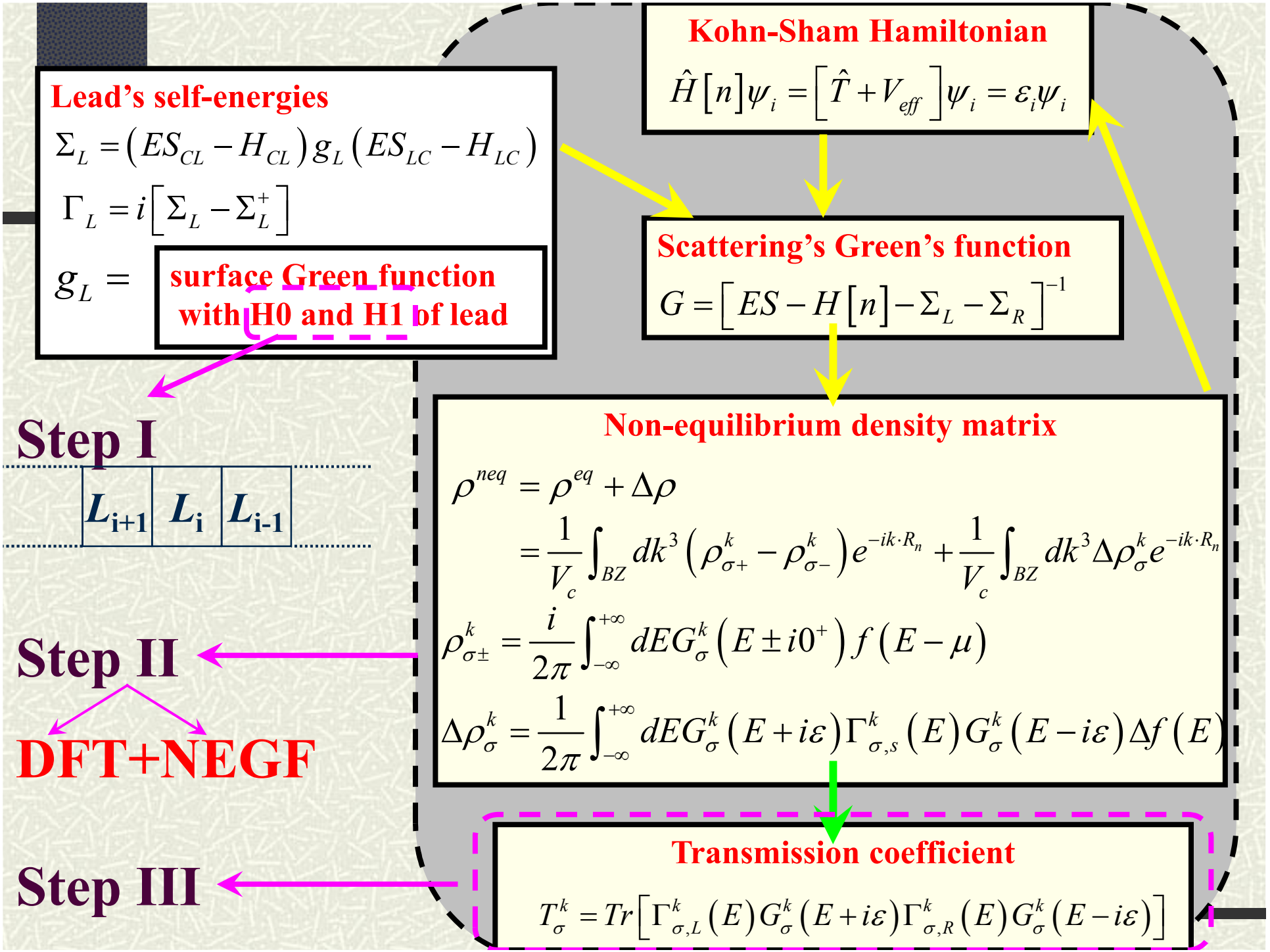
$$= \frac{1}{V_c}\int_{BZ} dk^3 \left(\rho^k_{\sigma+} - \rho^k_{\sigma-}\right) e^{-ik\cdot R_n} + \frac{1}{V_c}\int_{BZ} dk^3 \Delta\rho^k_\sigma e^{-ik\cdot R_n}$$

$$\rho^k_{\sigma\pm} = \frac{i}{2\pi}\int_{-\infty}^{+\infty} dE G^k_\sigma \left(E \pm i0^+\right) f\left(E - \mu\right)$$

$$\Delta\rho^k_\sigma = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dE G^k_\sigma \left(E + i\varepsilon\right)\Gamma^k_{\sigma,s}\left(E\right) G^k_\sigma \left(E - i\varepsilon\right)\Delta f\left(E\right)$$

Transmission coefficient

$$T^k_\sigma = Tr\left[\Gamma^k_{\sigma,L}\left(E\right) G^k_\sigma \left(E + i\varepsilon\right)\Gamma^k_{\sigma,R}\left(E\right) G^k_\sigma \left(E - i\varepsilon\right)\right]$$


Kohn-Sham Hamiltonian
$\hat{H}[n]\psi_i = \left[\hat{T} + V_{eff}\right]\psi_i = \varepsilon_i \psi_i$
Lead's self-energies
$\Sigma_L = (ES_{CL} - H_{CL})\, g_L\, (ES_{LC} - H_{LC})$
$\Gamma_L = i\left[\Sigma_L - \Sigma_L^+\right]$
$g_L =$ surface Green function with H0 and H1 of lead
Scattering's Green's function
$G = \left[ES - H[n] - \Sigma_L - \Sigma_R\right]^{-1}$
Step I
L_{i+1} L_i L_{i-1}
Non-equilibrium density matrix
$\rho^{neq} = \rho^{eq} + \Delta\rho$
$= \frac{1}{V_c}\int_{BZ} dk^3 \left(\rho^k_{\sigma+} - \rho^k_{\sigma-}\right) e^{-ik\cdot R_n} + \frac{1}{V_c}\int_{BZ} dk^3 \Delta\rho^k_\sigma e^{-ik\cdot R_n}$
Step II
$\rho^k_{\sigma\pm} = \frac{i}{2\pi}\int_{-\infty}^{+\infty} dE G^k_\sigma\left(E \pm i0^+\right) f(E-\mu)$
DFT+NEGF
$\Delta\rho^k_\sigma = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dE G^k_\sigma(E+i\varepsilon)\Gamma^k_{\sigma,s}(E) G^k_\sigma(E-i\varepsilon)\Delta f(E)$
Step III
Transmission coefficient
$T^k_\sigma = Tr\left[\Gamma^k_{\sigma,L}(E) G^k_\sigma(E+i\varepsilon)\Gamma^k_{\sigma,R}(E) G^k_\sigma(E-i\varepsilon)\right]$

Main structure of transport module

DFT.c

```
double DFT (……)
{
…
do {
Set_Aden_Grid (…);

Set_Hamiltonian (…, H, …);

 TRAN_DFT (…, H, S, …, DM, …);

Checking self-consistency;
} while (self-consistency)
…
}
```

TRAN_DFT.c

```
double TRAN_DFT (……)
{
…

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

TRAN_DFT_Kdependent(…k, … CDM,…);

}

Summing DM for all k-points;
…
}
```

$$\rho = \int_{BZ} dk^3 \rho^k$$

```
double DFT_Kdependent (…)
{
…

for (i=0;i<n_i;i++) {

E(i)=tran_omega_scf(i);
G^R, G^< and ρ;

}

…
}
```

$$\rho^k = \int_{-\infty}^{+\infty} dE G_\sigma^k(E)$$

DFT module

Kohn-Sham Hamiltonian

$$\hat{H}[n]\psi_i = \left[\hat{T} + V_{eff}\right]\psi_i = \varepsilon_i\psi_i$$

Main difference

$$V_C^H(\mathrm{r})\Big|_{z_L} = V_{L,bulk}^H(\mathrm{r})\Big|_{z_L}$$

$$V_C^H(\mathrm{r})\Big|_{z_R} = V_{R,bulk}^H(\mathrm{r})\Big|_{z_R}$$

```
if (Solver!=4 || TRAN_Poisson_flag2==4){
  FFT_Density(1,ReV1,ImV1,ReRhok[1][0],ImRhok[1][0]);
}
else{
  FFT2D_Density(1,ReV1,ImV1,ReRhok[1][0],ImRhok[1][0]);
}
```

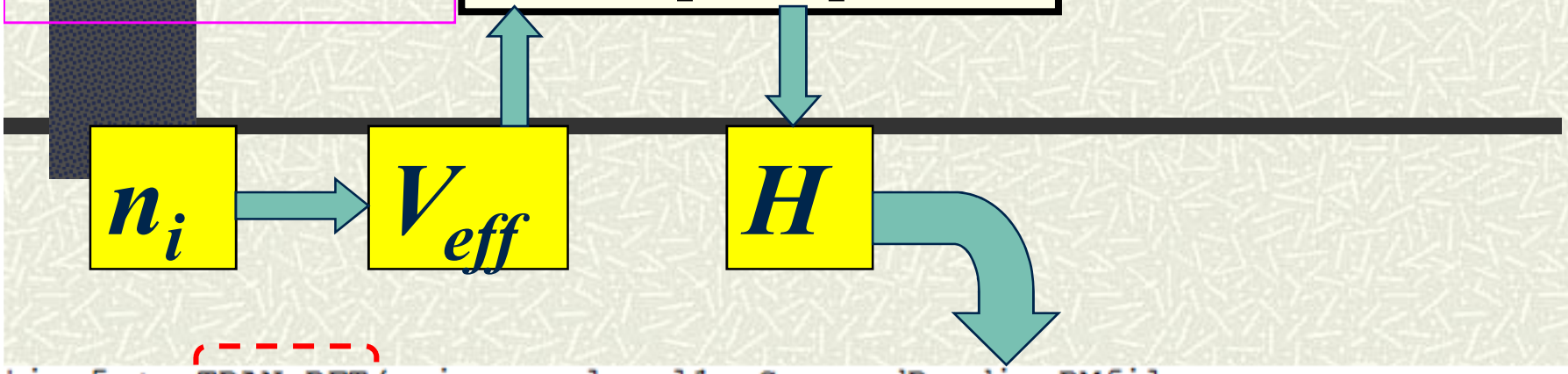
```
if (Solver!=4 && ESM_switch==0)       time4 += Poisson(1,ReV1,ImV1,ReV2,ImV2);
else if (Solver!=4 && ESM_switch!=0) time4 += Poisson_ESM(1,ReV1,ImV1,ReV2,ImV2);
else                                  time4 += TRAN_Poisson(ReV1,ImV1,ReV2,ImV2);
```

DFT.c

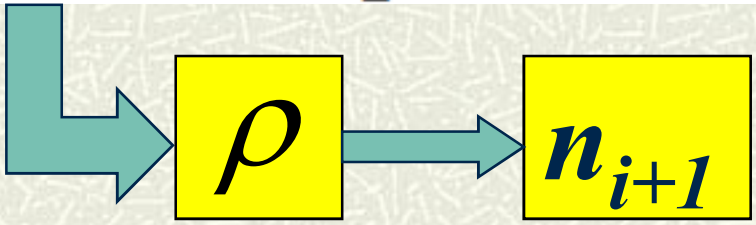
DFT module

Kohn-Sham Hamiltonian

$$\hat{H}[n]\psi_i = \left[\hat{T} + V_{eff}\right]\psi_i = \varepsilon_i \psi_i$$




```
time5 += TRAN_DFT(mpi_comm_level1, SucceedReadingDMfile,
                  level_stdout, LSCF_iter,SpinP_switch,H,iHNL,OLP[0],
                  atomnum,Matomnum,WhatSpecies, Spe_Total_CNO, FNAN, natn,ncn,
                  M2G, G2ID, F_G2M, atv_ijk, List_YOUSO,
                  DM[0],EDM,TRAN_DecMulP,Eele0,Eele1,ChemP_e0);
```



if (abs[n_i-n_{i+1}]<δ) {stop}

else {charge mixing; iterate}

DFT.c

NEGF module

The first 3 steps are not NEGF cal.

```
/*  if (TRAN_SCF_Iter_Band<iter || SucceedReadingDMfile==1){ */
 if (3<iter || SucceedReadingDMfile==1){

    TRAN_DFT_Original( comm1,
                       level_stdout,
                       iter,
                       SpinP_switch,
                       nh,    /* H */
                       ImNL, /* not used, s-o coupling */
                       CntOLP,
                       ........
                       ........
                       atv_ijk,
                       List_YOUSO,
                       /* output */
                       CDM,  /* output, density matrix */
                       TRAN_DecMulP, /* output, partial DecMulP */
                       ChemP_e0);
  }
```

NEGF calculation

```
  /*************************************************
    if SCF_iter<=3, employ the band diagonalization
  *************************************************/
  else {

    int i,j,k,n,n2,wanA;
```

Band calculation

TRAN_DFT.c

NEGF module

subroutine `double TRAN_DFT_Original`

$$\rho^{neq} = \rho^{eq} + \Delta\rho = \frac{1}{V_c}\int_{BZ} dk^3 \left(\rho^k_{\sigma+} - \rho^k_{\sigma-}\right) e^{-ik\cdot R_n} + \frac{1}{V_c}\int_{BZ} dk^3 \Delta\rho^k_{\sigma} e^{-ik\cdot R_n}$$

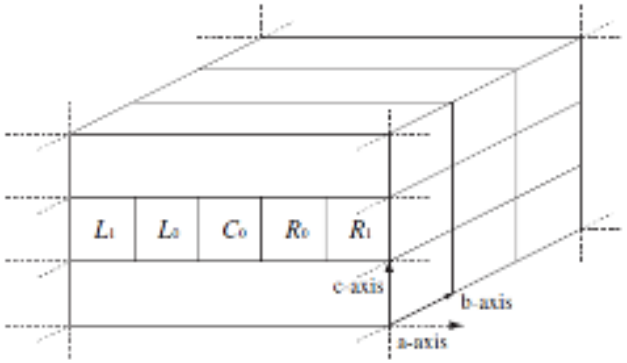
```
for (kloop0=0; kloop0<num_kloop0; kloop0++){

  kloop = S_knum + kloop0;

  k2 = T_KGrids2[kloop];
  k3 = T_KGrids3[kloop];
  k_op = T_op_flag[kloop];

    TRAN_DFT_Kdependent(MPI_CommWD1[myworld1],
                        parallel_mode, numprocs1, myid1,
                        level_stdout, iter, SpinP_switch,
                        k2, k3, k_op, order_GA,
                        DM1,H1,S1,
                        nh, ImNL, CntOLP,
                        atomnum, Matomnum, WhatSpecies,
                        Spe_Total_CNO, FNAN,
                        natn, ncn, M2G, G2ID, atv_ijk,
                        List_YOUSO, CDM, EDM, Eele0, E

} /* kloop0 */
```



TRAN_DFT.c

NEGF module

TRAN_DFT.c

subroutine `static void TRAN_DFT_Kdependent`

(1) Equilibrium part

T.Ozaki, PRB 75, 035123 (2007)

$$\rho^{k}_{\sigma\pm} = \frac{i}{2\pi}\int_{-\infty}^{+\infty} dE G^{k}_{\sigma}\left(E \pm i0^{+}\right) f\left(E-\mu\right) = \pm\frac{1}{4}\mu^{k,0}_{\sigma} \mp \frac{1}{\beta}\sum_{p}^{N_p} G^{k}_{\sigma}\left(\alpha_p\right) R_p$$

(2) Nonequilibrium part

$$\Delta f\left(E\right) = f\left(E-\mu_1\right) - f\left(E-\mu_2\right)$$

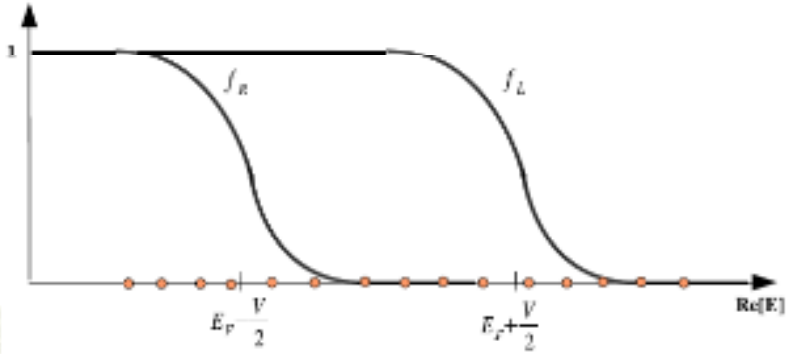
$$\Delta\rho^{k}_{\sigma} = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dE G^{k}_{\sigma}\left(E+i\varepsilon\right)\Gamma^{k}_{\sigma,s}\left(E\right) G^{k}_{\sigma}\left(E-i\varepsilon\right)\Delta f\left(E\right)$$

```
/*****************************************************************
          calculation of Green functions at k and iw
*****************************************************************/

for ( Miw=myid; Miw<tran_omega_n_scf*spinsize; Miw+=numprocs ) {

  k = Miw/tran_omega_n_scf;
  iw = Miw - k*tran_omega_n_scf;

  w = tran_omega_scf[iw];
  w_weight  = tran_omega_weight_scf[iw];
  iw_method = tran_integ_method_scf[iw];
```



NEGF module

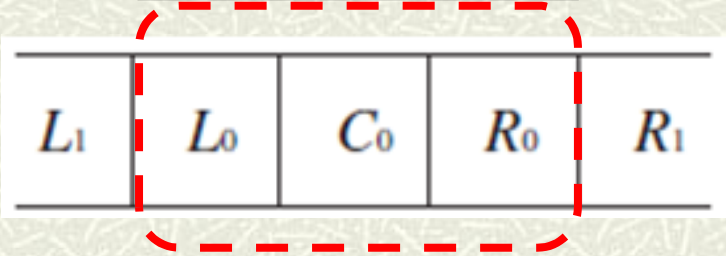
subroutine `static void TRAN_DFT_Kdependent`

Green function and self energy

$$G = \left[ES_{CC} - H_{CC} - \Sigma_L - \Sigma_R \right]^{-1}$$

$$\Sigma_R = \left(ES_{CR} - H_{CR} \right) g_L \left(ES_{RC} - H_{RC} \right)$$

Central region



Hamiltonian and overlap matrix

```
/* set Hamiltonian and overlap matrices of left and right leads */

TRAN_Set_SurfOverlap(comm1,"left", k2, k3);
TRAN_Set_SurfOverlap(comm1,"right",k2, k3);

/* set CC, CL and CR */

TRAN_Set_CentOverlap(   comm1,
                        3,
                        SpinP_switch,
                        k2,
                        k3,
```

TRAN_DFT.c

NEGF module

subroutine `static void TRAN_DFT_Kdependent`

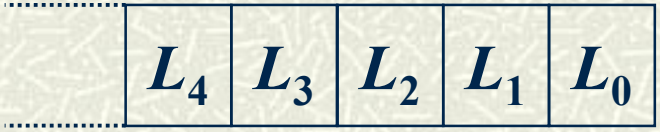
Retarded terms

$$G = \left[ES_{CC} - H_{CC} - \Sigma_L - \Sigma_R \right]^{-1}$$

$$\Sigma_L = \left(ES_{CR} - H_{CR} \right) g_L \left(ES_{RC} - H_{RC} \right)$$

surface Green function g_L

M.P.L.Sancho, JPF 15,851 (1985)




```
/* calculation of surface Green's function and self energy from the RIGHT lead */

iside = 1;

TRAN_Calc_SurfGreen_direct(w, NUM_e[iside], H00_e[iside][k], H01_e[iside][k],
                           S00_e[iside], S01_e[iside], tran_surfgreen_iteration_max,
                           tran_surfgreen_eps, GRR);

TRAN_Calc_SelfEnergy(w, NUM_e[iside], GRR, NUM_c, HCR[k], SCR, SigmaR);

/* calculation of central retarded Green's function */

TRAN_Calc_CentGreen(w, NUM_c, SigmaL, SigmaR, HCC[k], SCC, GC);
```

TRAN_DFT.c

NEGF module

TRAN_DFT.c

subroutine `static void TRAN_DFT_Kdependent`

Advanced terms

$$G = \left[ES_{CC} - H_{CC} - \Sigma_L - \Sigma_R \right]^{-1}$$

```
if (TRAN_Kspace_grid2==1 && TRAN_Kspace_grid3==1 && iw_method==2){

  for (i=0; i<NUM_c*NUM_c; i++) {
    SigmaL_Ad[i].r = SigmaL[i].r;
    SigmaL_Ad[i].i =-SigmaL[i].i;
    SigmaR_Ad[i].r = SigmaR[i].r;
    SigmaR_Ad[i].i =-SigmaR[i].i;
    GC_Ad[i].r = GC[i].r;
    GC_Ad[i].i =-GC[i].i;
  }
  TRAN_Calc_CentGreenLesser (.........);
}
/* in case of TRAN_Kspace_grid2!=1 || TRAN_Kspace_grid3!=1 */
/* calculation of advanced Green's function */
else if (iw_method==2){

 /* conjugate complex */
  w.i = -w.i;

  /* calculation of surface Green's function and self energy from the LEFT lead */
  iside = 0;
  TRAN_Calc_SurfGreen_direct(w, NUM_e[iside], H00_e[iside][k], H01_e[iside][k],
                             S00_e[iside], S01_e[iside], tran_surfgreen_iteration_max,
                             tran_surfgreen_eps, GRL);
```

$k = 0:$ $\quad G^A = \left(G^R \right)^*$

$k \neq 0:$ $\quad G^A = G\left(E - i\varepsilon \right)$

NEGF module

TRAN_DFT.c

subroutine `static void TRAN_DFT_Kdependent`

(1) Equilibrium part

$$\rho^{k}_{\sigma\pm} = \pm\frac{1}{4}\mu^{k,0}_{\sigma} \mp \frac{1}{\beta}\sum_{p}^{N_p} G^{k}_{\sigma}(\alpha_p)R_p$$

(2) Nonequilibrium

$$\Delta\rho^{k}_{\sigma} = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dE G^{k}_{\sigma}(E+i\varepsilon)\Gamma^{k}_{\sigma,s}(E)G^{k}_{\sigma}(E-i\varepsilon)\Delta f(E)$$

```
if (iw_method==1)
  TRAN_Add_MAT( 1, NUM_c, w_weight, GC,     v2[k]);
else if (iw_method==2)
  TRAN_Add_MAT( 1, NUM_c, w_weight, Gless,  v2[k]);
```

```
kRn = k2*(double)l2 + k3*(double)l3;
si = (double)k_op*sin(2.0*PI*kRn);
co = (double)k_op*cos(2.0*PI*kRn);

for (i=0; i<tnoA; i++) {
  for (j=0; j<tnoB; j++) {
    re = v3[itot++];
    im = v3[itot++];

    /* divided by numprocs due to the later MPI_Allreduce  */
    DM1[k][itot0++] += (re*co + im*si)/(double)numprocs;
```

$$\rho = \frac{1}{V_c}\int_{BZ} dk^3 \left(\rho^{k}_{\sigma+} - \rho^{k}_{\sigma-}\right)e^{-ik\cdot R_n} + \frac{1}{V_c}\int_{BZ} dk^3 \Delta\rho^{k}_{\sigma} e^{-ik\cdot R_n}$$

NEGF module

TRAN_DFT.c

subroutine `double TRAN_DFT_Original`

$$\rho = \frac{1}{V_c}\int_{BZ} dk^3 \left(\rho^k_{\sigma+} - \rho^k_{\sigma-}\right) e^{-ik\cdot R_n} + \frac{1}{V_c}\int_{BZ} dk^3 \Delta\rho^k_{\sigma} e^{-ik\cdot R_n}$$

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

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

    TRAN_DFT_Kdependent(.......,DM1,....);
} /* kloop0 */

/* MPI communication of DM1 */

tmp = 1.0/(double)(TRAN_Kspace_grid2*TRAN_Kspace_grid3);

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

  MPI_Allreduce( DM1[k], TDM1, size_H1, MPI_DOUBLE, MPI_SUM, comm1);
```

```
if (1<=MA_AN && MA_AN<=Matomnum){
  CDM[k][MA_AN][LB_AN][i][j] = TDM1[itot0]*tmp;
}
```

ρ

Return the new density matrix ρ to DFT module

Thank you !