PWmat-TDDFT Manual & TEST

0.PWmat

1.JOB=TDDFT

support:

xcfunctional=lda/pbe
norm conserving psedupotential

2.TDDFT_DETAIL=m1 m2 mstate

default: TDDFT_DETAIL=1 NUM_BAND NUM_BAND

description:

Expand \psi_j(t) in terms of the adiabatic eigenstates \phi_i:
\psi_j(t)=\sum_i C_ji(t)\phi_i(t)
Define the *Adiabatic window* [m1,m1+m2-1],
\psi_j(t)=\phi_j(t), j=1,m1-1
\psi_j(t)=\sum_i C_ji(t)\phi_i(t), j=m1,mstate+m1-1; i=1,m1+m2-1

[m1,m1+m2-1]	Adiabatic window, the [1,m1-1] will always be occupied by the first [1,m1-1] \psi_j,{j=1,m1-1} state.	\phi_i,i=m1,m1+m2-1	1<=m1+m2-1<=NUM_BAND
[1,msate]	Wavefunction index	\psi_j,j=1,mstate+m1-1	1<=msate<=m2

how to choose the parameters:

[m1,m2]
mstate

example1:

atom.config:

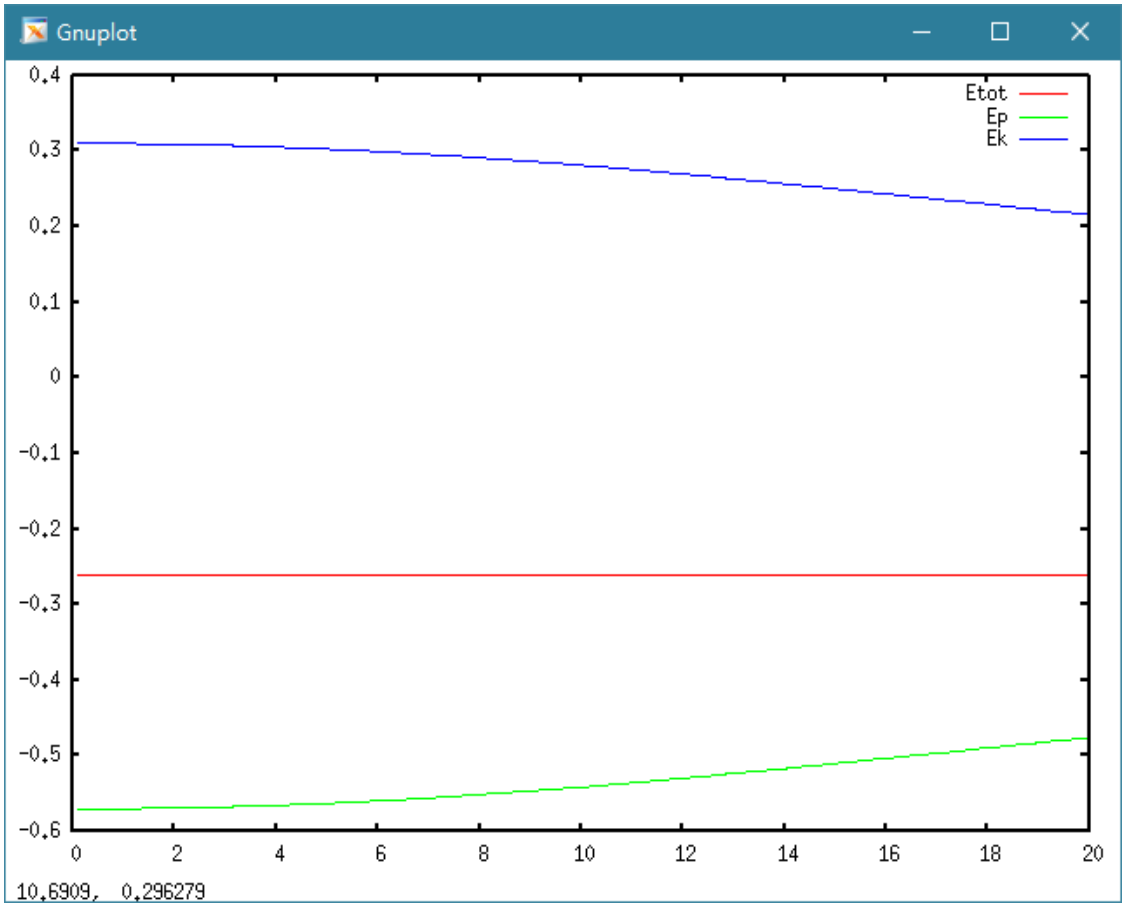
```
8

Lattice vector

5.65     0.00     0.00
```

```
  0.00     5.65     0.00

  0.00     0.00     5.65

Position, move_x, move_y, move_z

31   0.001000000000   0.000000000000   0.000000000000  1  1  1   1.0

31   0.000000000000   0.501000000000   0.502000000000  1  1  1   1.0

31   0.500000000000   0.000000000000   0.500000000000  1  1  1   1.0

31   0.500000000000   0.500000000000   0.000000000000  1  1  1   1.0

33   0.250000000000   0.250000000000   0.250000000000  1  1  1   0.0

33  -0.250000000000  -0.250000000000   0.250000000000  1  1  1   0.0

33  -0.250000000000   0.250000000000  -0.250000000000  1  1  1   0.0

33   0.250000000000  -0.250000000000  -0.250000000000  1  1  1   0.0
```

default settings:

```
1          1

IN.ATOM   = atom.config

JOB       = TDDFT

MD_DETAIL = 1, 200, 0.1, 300,300

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF
```

Etot,Ek,Ep plot:



example2:

use adiabatic window:

from the output file OUT.OCC of example1:

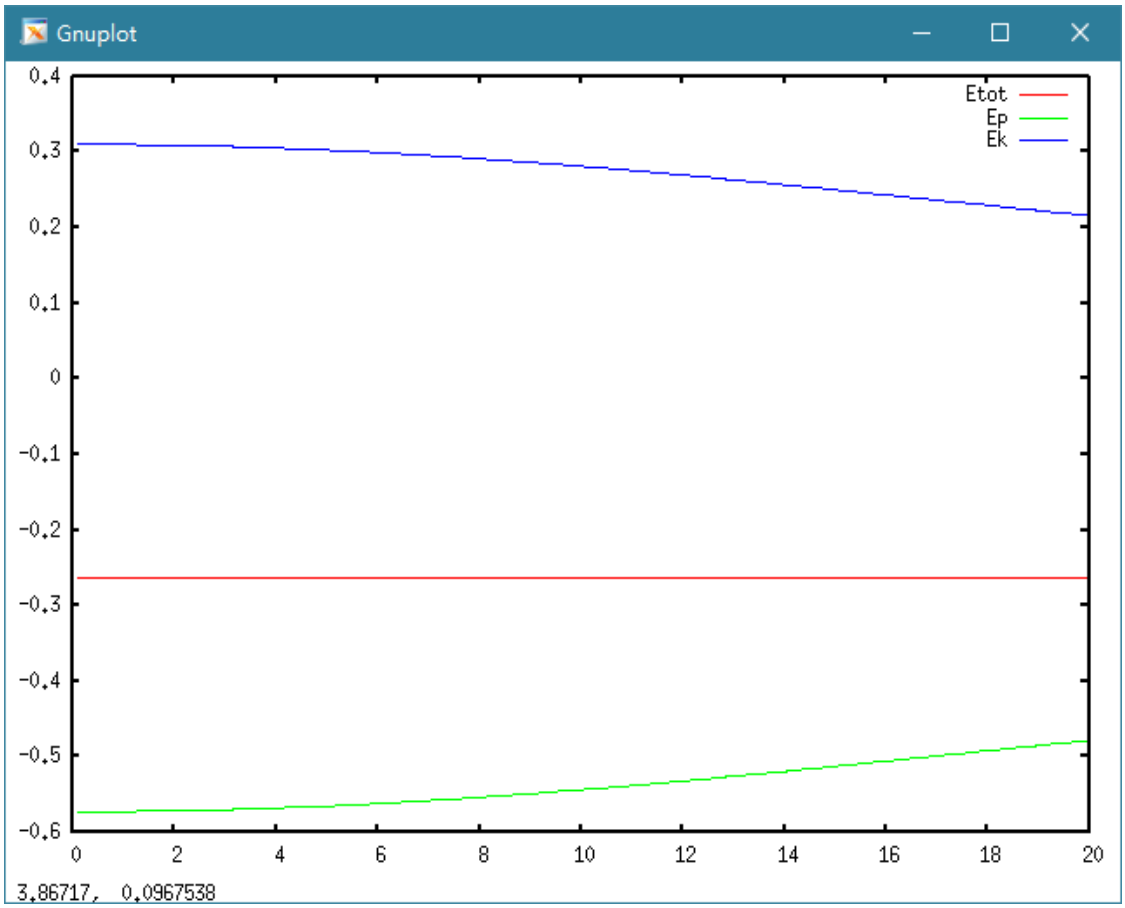
```
KPOINTS   1:   0.0000   0.0000   0.0000

NO.   ENERGY(eV) OCCUPATION

 1   -10.7422   2.00000

 2    -8.3784   2.00000

 3    -8.2272   2.00000

 4    -8.1217   2.00000

 5    -5.0553   2.00000

 6    -5.0473   2.00000

 7    -5.0042   2.00000

 8    -0.8431   2.00000

 9    -0.8061   2.00000
```

```
10    -0.7368   2.00000

11    -0.7011   2.00000

12    -0.6666   2.00000

13    -0.6165   2.00000

14     1.8319   1.99983

15     2.0285   1.99966

16     2.1978   1.99956

17     2.4204   0.00095

18     3.0161   0.00000

19     3.0985   0.00000

20     3.2698   0.00000

21     3.3809   0.00000

22     3.4191   0.00000

23     3.5045   0.00000

24     5.4035   0.00000

25     5.5223   0.00000

26     5.6578   0.00000
```

we know that the [1,16] states are occupied, and total num of band is 26. Then we can set the TDDFT_DETAIL=m1 m2 mstate,**m1 \in [1,16], m2 \in [1,26-m1], mstate \in [1,m2]**

```
1         1

IN.ATOM   = atom.config

JOB       = TDDFT

MD_DETAIL = 1, 200, 0.1, 300,300

TDDFT_DETAIL=6,20,16

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF
```

Etot,Ep,Ek plot:



3.OUT.TDDFT=T1 T2 n1 T3 n2

default: OUT.TDDFT=F F 100 F 100

description:

The output files can be used to **restart** TDDFT and show the process of TDDFT.

T1,T2,n1	T1=T/F	eigen energy, dipole, occ(i) per n1 steps	the output will be in file OUT.TDDFT1. One can use plot_TDDFT.f to read and output OUT.TDDFT1.
	T2=T/F	Cij per n1 steps	
T3,n2	T3=T/F	output all the wavefunctions and charge densities per n2 steps for restart.	the output will be in file OUT.TDDFT,OUT.WG,OUT.RHO and directory TDDOS/. This can be very expensive, so use large n2.

example3:

```
 1       1

IN.ATOM  = atom.config

JOB      = TDDFT
```

```
MD_DETAIL = 1, 200, 0.1, 300,300

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF

Ecut      =   30

N123      =   32   32   32

OUT.TDDFT = T T 10 T  50
```

ls:

./	OUT.TDDFT1	update per 10 steps	used by plot_TDDFT.f
./	OUT.WG OUT.RHO OUT.TDDFT	update per 50 steps	used by restarting TDDFT
TDDOS	OUT.WG.0.100000 TDEIGEN.0.100000 OUT.EIGEN.0.100000 OUT.WG.5.000000 TDEIGEN.5.000000 OUT.EIGEN.5.000000 OUT.WG.10.000000 OUT.EIGEN.10.000000 TDEIGEN.10.000000 OUT.WG.15.000000 OUT.EIGEN.15.000000 TDEIGEN.15.000000 OUT.WG.20.000000 TDEIGEN.20.000000 OUT.EIGEN.20.000000	update per 50 steps	used by ploting DOS

4.TDDFT_SPACE=itype1, N, a(1),...,a(N)

default:TDDFT_SPACE=0 N a(1) ... a(N)

description:

This controls the real space Vext_tddft(r). Vext_tddft(r) refers to the external potential in real space for tddft calculation.

itype1	0	no external input term.		
	1	read vext_tddft from file IN.VEXT_TDDFT(all capital, same format as in IN.VEXT)		
	2	Vext_tddft(r)=(x-x0)a(1)+(x-x0)^2a(2)+(y-y0)a(3)+(y-y0)^2a(4)+(z-z0)a(5)+(z-z0)^2a(6), (x0,y0,z0) is center of AL box.	all a(i) atomic unit	output file OUT.VEXT_TDDFT
	3	Vext_tddft(r)=a(1)exp{-[(x-x0)^2+(y-y0)^2+(z-z0)^2]/a(2)^2}	a(1) Hartree unit, a(2) Bohr unit	output file OUT.VEXT_TDDFT
	-1	Not use real space format, but use G-space,it wil use IN.A_FIELD		

example6:

itype1=1.

first we can get IN.VEXT_TDDFT by set **ityp1=2**. [Vext_tddft(r)=(x-

x0)*0.002，**不随时间变化**]

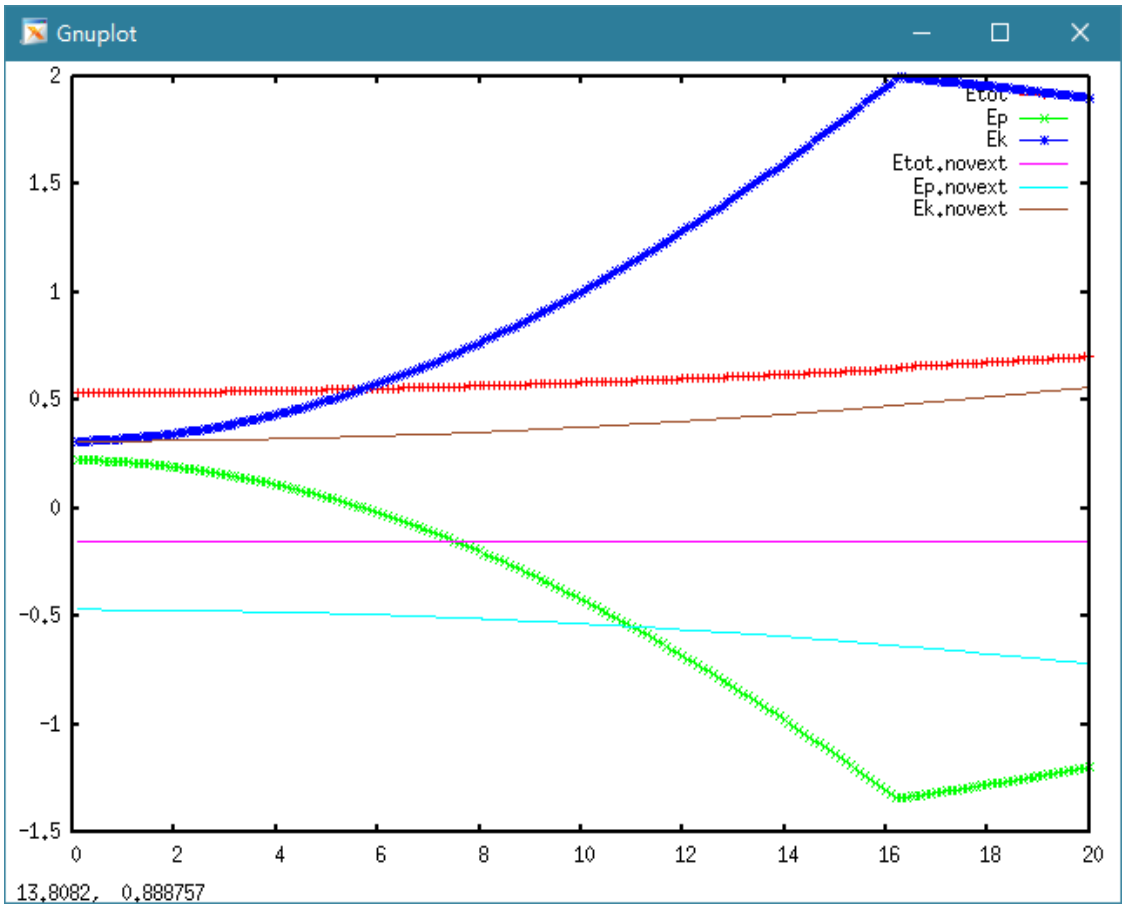
```
1          1

IN.ATOM   = atom.config

JOB       = TDDFT

precision = double

convergence=difficult

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF

MD_DETAIL = 1, 200, 0.1, 300,300

TDDFT_DETAIL = 1,30,30

TDDFT_SPACE = 2, 6, 0.002,0.0,0.0,0.0,0.0,0.0

OUT.TDDFT = T T 5 T 10

XCFUNCTIONAL = PBE

num_band  =  30

Ecut      =   30.0

N123      = 32 32 32
```

```
cp OUT.VEXT_TDDFT IN.VEXT_TDDFT
```

```
1          1

IN.ATOM   = atom.config

JOB       = TDDFT

precision = double

convergence=difficult

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF
```

```
MD_DETAIL = 1, 200, 0.1, 300,300

TDDFT_DETAIL = 1,30,30

TDDFT_SPACE = 1, 6, 0.002,0.0,0.0,0.0,0.0,0.0

OUT.TDDFT = T T 5 T 10

XCFUNCTIONAL = PBE

num_band  =  30

Ecut      =   30.0

N123      = 32 32 32
```

Etot,Ep,Ek plot:



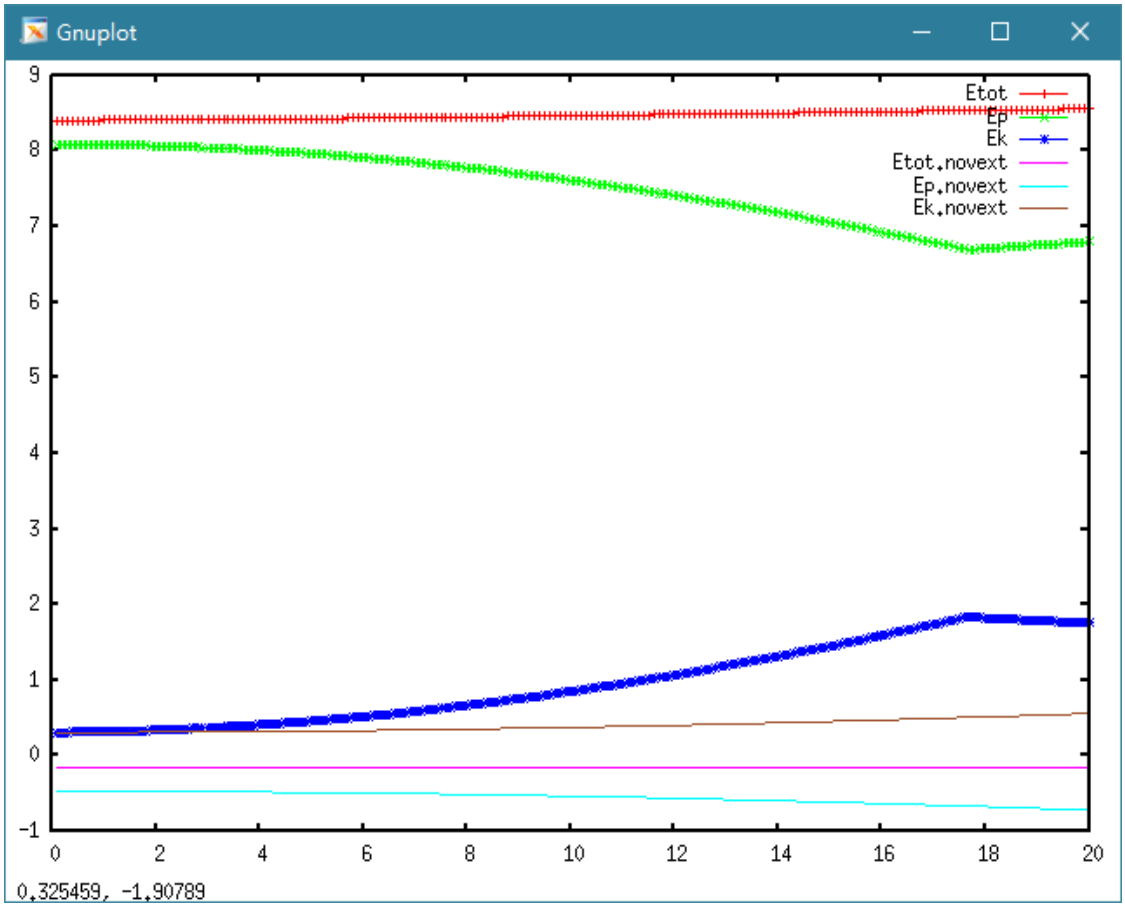
example7:

itype1=2.[Vext_tddft(r)=(x-x0)*0.002+(x-x0)^2*0.001，不随时间变化]

```
1        1
```

```
IN.ATOM   = atom.config

JOB       = tddft

precision = double

convergence=difficult

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF

MD_DETAIL = 1, 200, 0.1, 300,300

TDDFT_DETAIL = 1,30,30

TDDFT_SPACE = 2, 6, 0.002,0.001,0.0,0.0,0.0,0.0

OUT.TDDFT = T T 5 T 10

XCFUNCTIONAL = PBE

num_band  =  30

Ecut      =   30.0

N123      = 32 32 32
```

Etot,Ep,Ek plot:



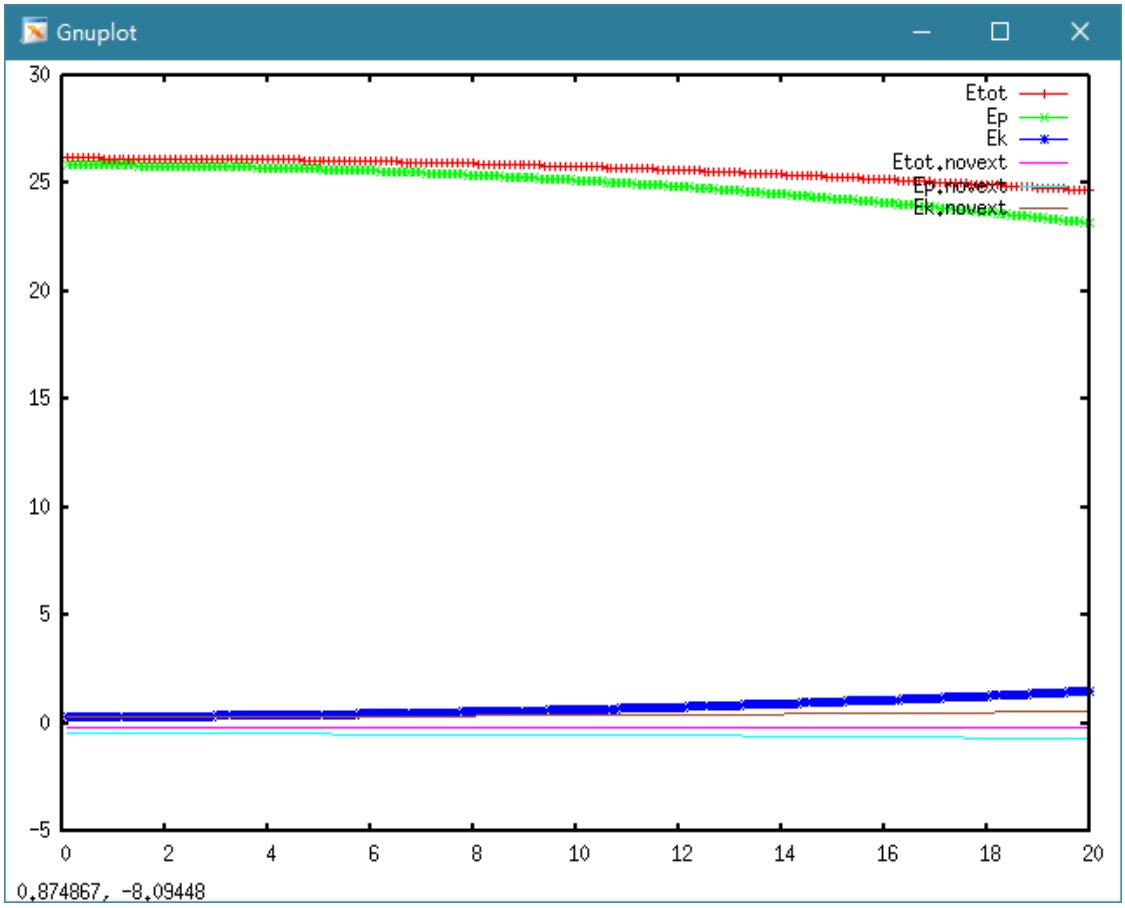
example8:

itype1=3.[Vext_tddft(r)=1.0*exp{-[(x-x0)^2+(y-y0)^2+(z-z0)^2]/2.0^2}，不随时间变化]

```
1        1

IN.ATOM   = atom.config

JOB       = tddft

precision = double

convergence=difficult

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF

MD_DETAIL = 1, 200, 0.1, 300,300

TDDFT_DETAIL = 1,30,30

TDDFT_SPACE = 3, 2, 1.0,2.0

OUT.TDDFT = T T 5 T 10
```

```
XCFUNCTIONAL = PBE

num_band  =  30

Ecut      =   30.0

N123      = 32 32 32
```

Etot,Ep,Ek plot:



itype1=-1. ref. IN_A.FIELD.

5.IN.A_FIELD=T/F,a_field1,a_field2,a_field3

default: IN.A_FIELD=F 0.0 0.0 0.0

description:

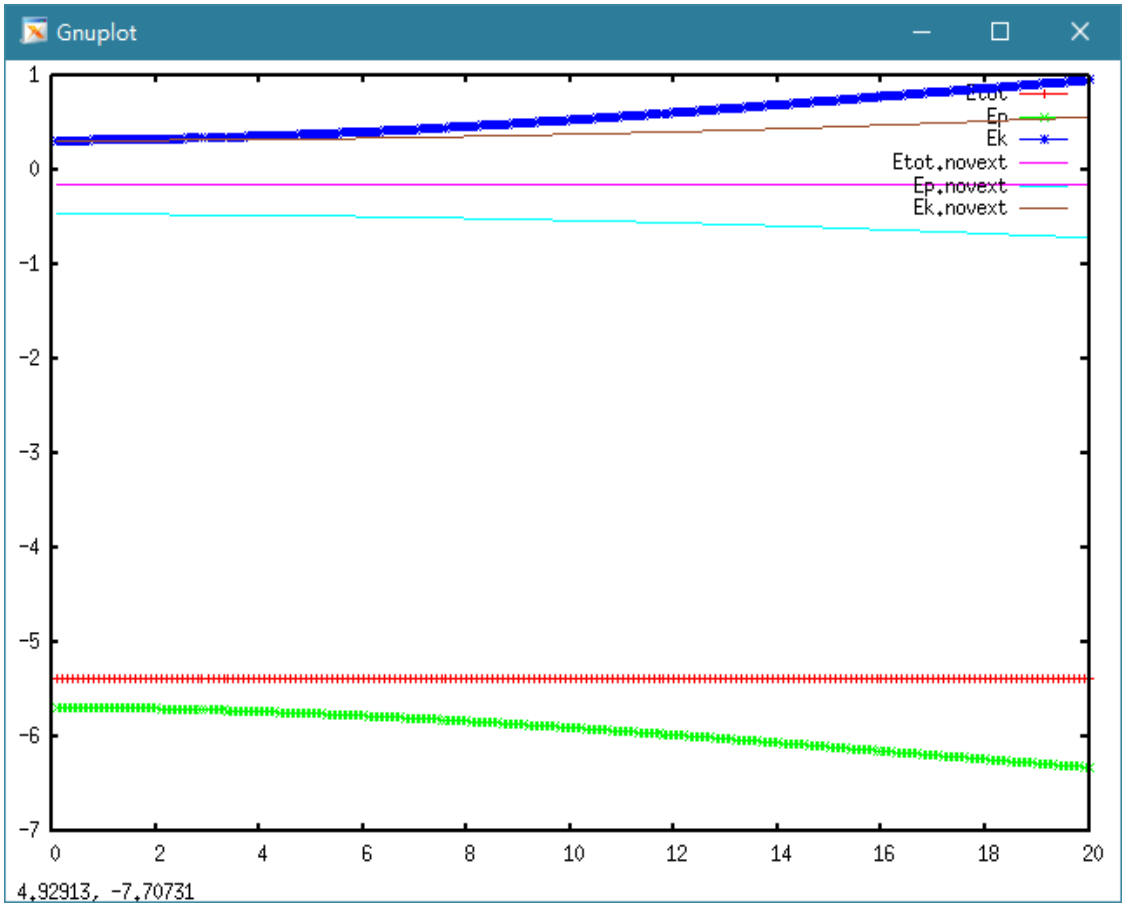
This controls the G-sapce external potential input for tddft calculation.(only used when **TDDFT_SPACE=-1,...**;)
the tddft hamiltonian

$$H=-1/2\ (\lap_x + i\ a\_field1)^2+1/2(\lap_y+ i\ a\_field2)^2+1/2(\lap_z + i\ a\_field3)^3$$

example9:

```
1          1

IN.ATOM   = atom.config

#precision = double

JOB       = TDDFT

precision = double

convergence=difficult

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF

MD_DETAIL = 1, 200, 0.1, 300,300

TDDFT_DETAIL = 1,30,30

TDDFT_SPACE = -1,6, 0.002,0,0.,0, 0., 0

IN.A_FIELD = T  0.1 0.2 0.3

OUT.TDDFT = T T 5 T 10

XCFUNCTIONAL = PBE

Ecut      =   30.0

num_band  =  30

N123      = 32 32 32
```

Etot,Ep,Ek plot:



6.TDDFT_TIME=itype2,N,b(1),...,b(N)

default: TDDFT_TIME=0 N b(1) ... b(N)

description:

This is used to control the time dimension of the external function fTDDFT(i).

itype2	0	ftddft(t)=1.0		
	1	read in ftddft(i) from IN.TDDFT_TIME	file likes: 0 ftddft(0) 1 ftddft(1) ... N ftddft(N)	note: N+1 lines
	2	ftddft(t)=b(1)exp(-(t-b(2))^2/b(3)^2)sin(b(4)t+b(5))	b(2),b(3) fs unit	output OUT.TDDFT_TIME

For TDDFT Hamiltonian, we have:

itype1	.ne. -1	H(t)=H0+Vext_tddft(r)ftddft(t)
	-1	H(t)=-1/2(\lap_x+i A_x*ftddft(t))-1/2(\lap_y+i A_y*ftddft(t))^2-1/2(\lap_z+i A_z*ftddft(t))^2

example10:

itype1=2,itype2=1.

```
1        1

IN.ATOM   = atom.config
```

```
JOB       = TDDFT

precision = double

convergence=difficult

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF

MD_DETAIL = 1, 200, 0.1, 300,300

TDDFT_DETAIL = 1,30,30

TDDFT_SPACE = 2, 6, 0.002,0,0.,0, 0., 0

TDDFT_TIME = 1, 5, 1.d0,5.,3., 1.5, 0.0

OUT.TDDFT = T T 5 T 10

XCFUNCTIONAL = PBE

Ecut      =   30.0

num_band  =  30

N123      = 32 32 32
```

IN.TDDFT_TIME

```
         0  0.000000000000000E+000

         1  1.037194639886028E-002

         2  2.284511287170516E-002

         3  3.736828505828689E-002

         4  5.378968011195755E-002

         5  7.184419673777015E-002

         6  9.114384810445718E-002

         7  0.111172445929042

         8  0.131285553886038

         9  0.150716610764225
```

10 0.168589934786881

11 0.183941060535575

12 0.195744533878874

13 0.202948908060838

14 0.204518260513532

15 0.199479104609557

16 0.186971127121559

17 0.166299767308467

18 0.136988295682909

19 9.882677803029927E-002

20 5.191514970317339E-002

21 -3.302400641857682E-003

22 -6.601441283612834E-002

23 -0.135032890361858

24 -0.208799727682720

25 -0.285410166808150

26 -0.362653885250895

27 -0.438073478988510

28 -0.509039200452352

29 -0.572837888962477

30 -0.626773140546486

31 -0.668272959157753

32 -0.695000464454575

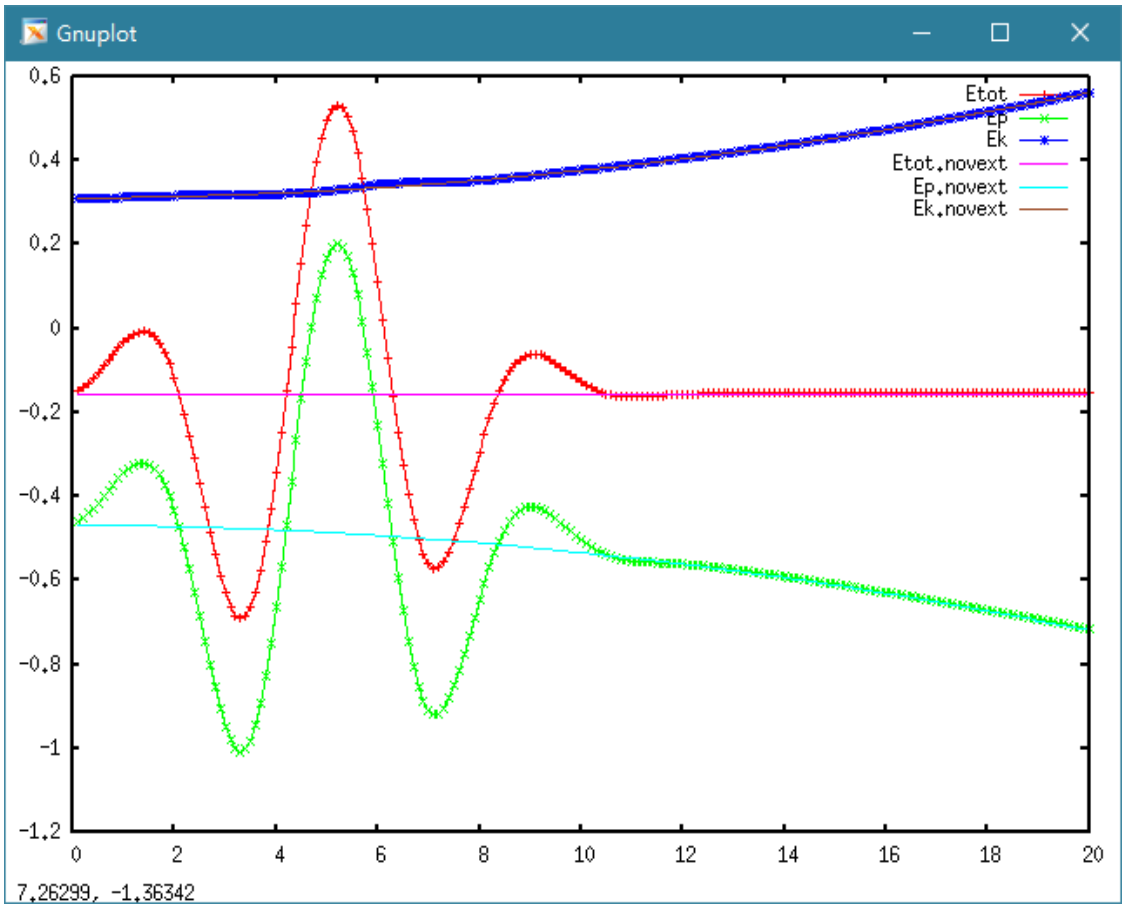
33 -0.704962750706460

34 -0.696612737562989

....

```
195 -5.921998502932264E-011

196 -4.671431218955184E-011

197 -3.575974730194868E-011

198 -2.664695193942652E-011

199 -1.936043364608484E-011

200 -1.372172773221090E-011
```

Etot,Ep,Ek plot:



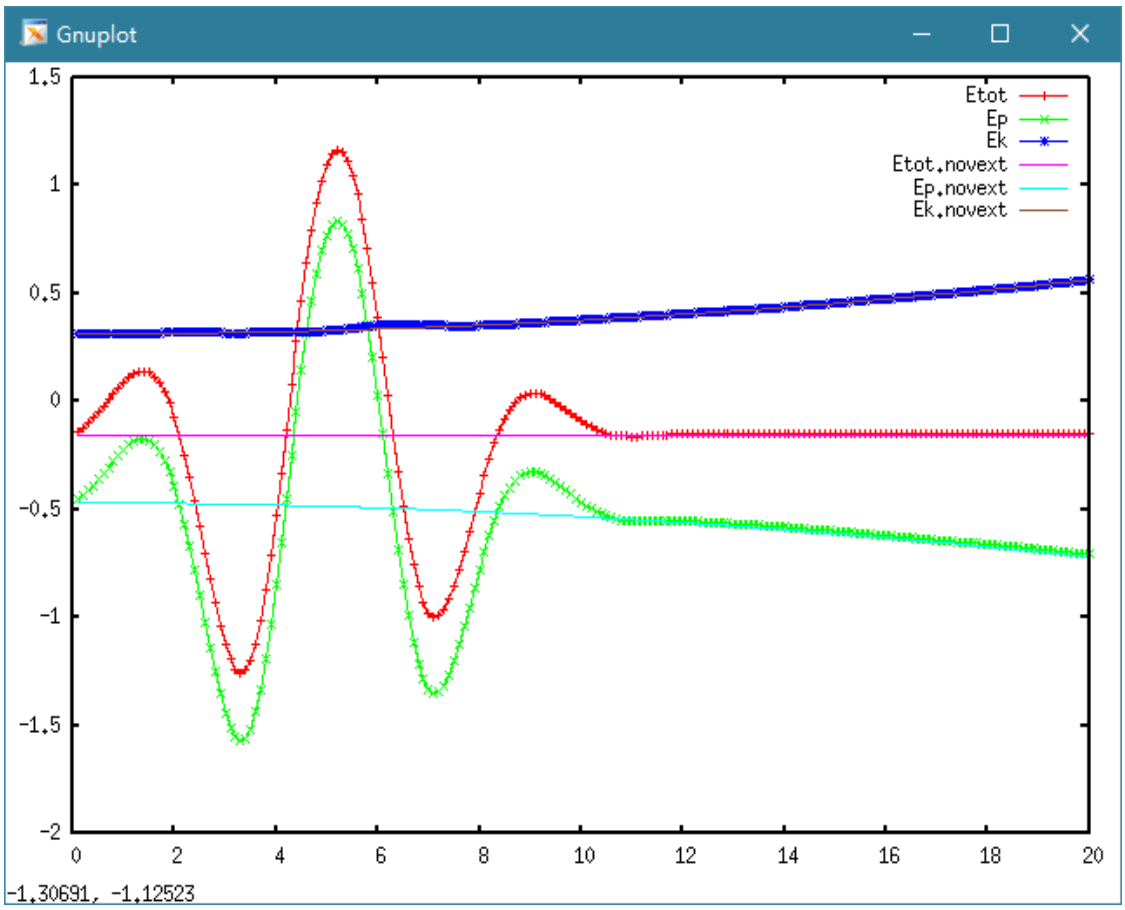
example11:

itype1=2,itype2=2.

```
1         1

IN.ATOM   = atom.config

JOB       = TDDFT

precision = double
```

```
convergence=difficult

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF

MD_DETAIL = 1, 200, 0.1, 300,300

TDDFT_DETAIL = 1,30,30

TDDFT_SPACE = 2, 6, 0.002,0,0.,0, 0., 0

TDDFT_TIME = 2, 5, 2.d0,5.,3., 1.5, 0.0

OUT.TDDFT = T T 5 T 10

XCFUNCTIONAL = PBE

Ecut      =   30.0

num_band  =  30

N123      = 32 32 32
```

Etot,Ep,Ek plot:

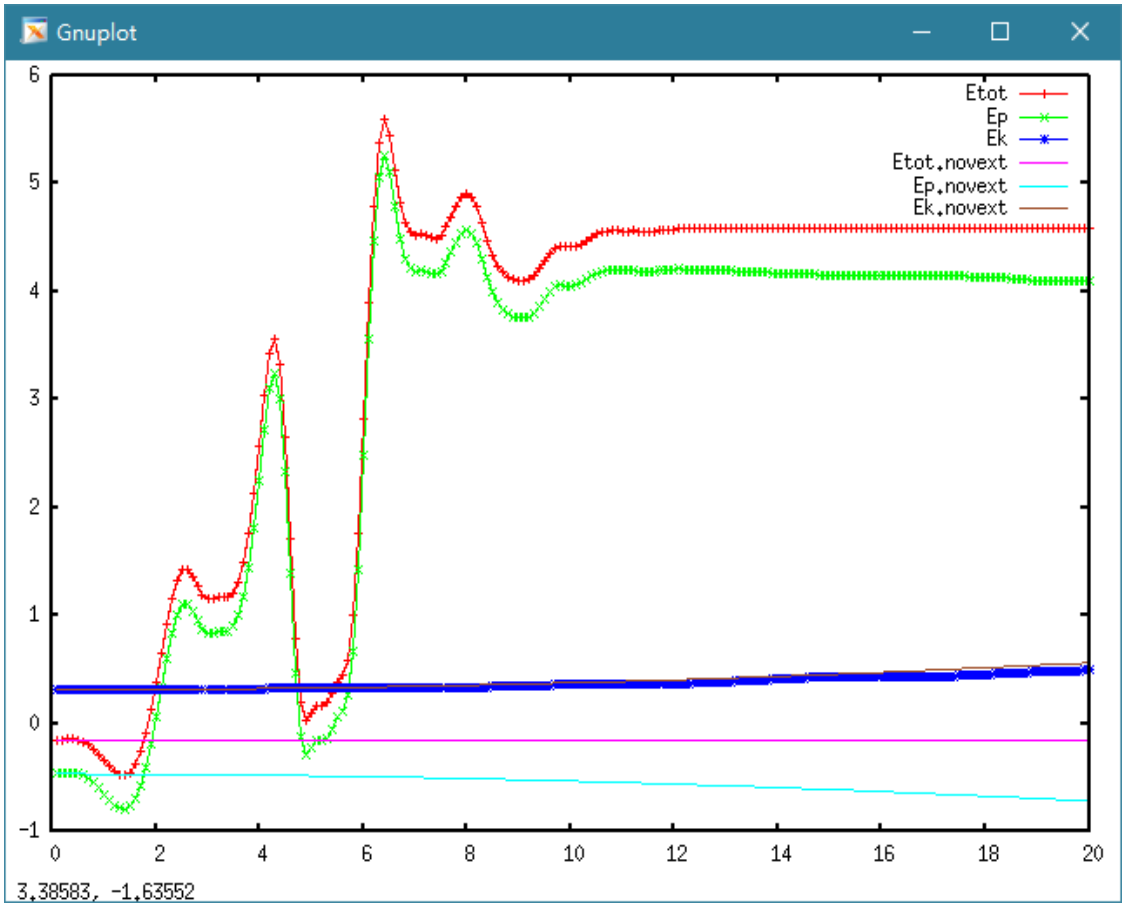


example12:

itype1=-1,itype2=2.

```
1          1

IN.ATOM   = atom.config

JOB       = TDDFT

precision = double

convergence=difficult

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF

MD_DETAIL = 1, 200, 0.1, 300,300

TDDFT_DETAIL = 1,30,30

TDDFT_SPACE = -1, 6, 0.002,0,0.,0, 0., 0

IN.A_FIELD = T  0.1 0.0 0.0

TDDFT_TIME = 2, 5, 2.d0,5.,3., 1.5, 0.0

OUT.TDDFT = T T 5 T 10

XCFUNCTIONAL = PBE

Ecut      =   30.0

num_band  =  30

N123      = 32 32 32
```

Etot,Ep,Ek plot:



7.IN.OCC/IN.OCC_2

description:

The **files** are used to set the ocupation of adiabatic eigenstates when **FERMI-DIRAC=0**.

spin=1, use IN.OCC
spin=2, use both IN.OCC and IN.OCC_2

File looks like:

```
1.0 1.0 1.0 0.6 0.0 0.0 0.0 ... ------occupations for k-point1

1.0 1.0 1.0 0.6 0.0 0.0 0.0 ... ------occupations for k-point2

  ....
```

example13:

etot.input

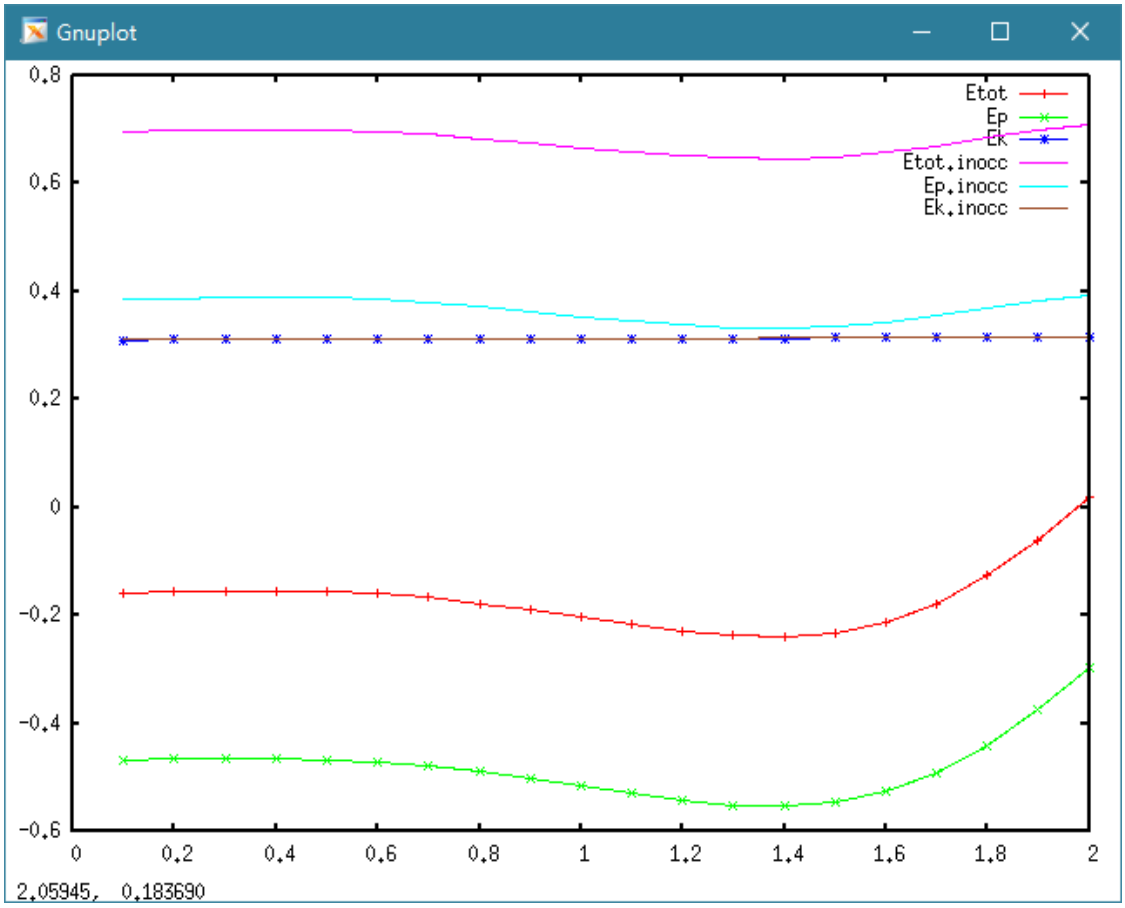
```
 1        1

 IN.ATOM   = atom.config

 IN.PSP1   = 31-Ga.LDA.fhi.UPF
```

```
IN.PSP2   = 33-As.LDA.fhi.UPF

precision = double

convergece=difficult

JOB       = TDDFT

MD_DETAIL = 1, 20, 0.1, 300,300

TDDFT_DETAIL = 1,30,30

TDDFT_SPACE = -1,6, 0.002,0,0.,0, 0., 0

TDDFT_TIME = 2, 5, 1.d0,5.,3., 1.5, 0.0

OUT.TDDFT = T T 5 T 10

XCFUNCTIONAL = PBE

IN.A_FIELD = T  0.1 0.0 0.0

Ecut      =   30.0

num_band  =  30

N123     = 32 32 32

SCF_ITER0_1 =    6   4    3    0.0000     0.02500   0

SCF_ITER0_2 =   94   4    3    1.0000     0.02500   0
```

IN.OCC

```
1 1 1 1 1 1 1 1 1 1

1 1 1 0.66666666666666

0.66666666666666 0.66666666666666 1

0 0 0 0 0 0 0 0 0 0 0 0
```

Etot,Ep,Ek plot:



8.IN.CC/IN.CC_2

description:

The **files** are used to initialize the **Cij** for TDDFT when **FREMI-DIRAC=-1**, which is used as ***\psi_j(t)=\sum_i C_ji(t)\phi_i(t)***.

spin=1, use IN.CC
spin=2, use both IN.CC and IN.CC_2

File looks like:

```
1  1  1.0

1  2  1.0

1  3  1.0

2  4  0.8  5 0.2

1  5  1.0

....
```

Line **j** specify the **psi_j, j=1,mstate**.
Define pair **(i,CC)**, **i** is the index of adiabatic states, **CC** is the value of **Cji**.
The first column specify the number of pairs.

If **m**, one index of adiabatic states, is not specified , then **Cjm=0**.

example14:

etot.input

```
1          1

IN.ATOM   = atom.config

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF

precision = double

convergece=difficult

JOB       = TDDFT

MD_DETAIL = 1, 20, 0.1, 300,300

TDDFT_DETAIL = 1,30,30

TDDFT_SPACE = -1,6, 0.002,0,0.,0, 0., 0

TDDFT_TIME = 2, 5, 1.d0,5.,3., 1.5, 0.0

OUT.TDDFT = T T 5 T 10

XCFUNCTIONAL = PBE

IN.A_FIELD = T  0.1 0.0 0.0

Ecut      =   30.0

num_band  =  30

N123      = 32 32 32

SCF_ITER0_1 =    6   4    3    0.0000     0.02500   -1

SCF_ITER0_2 =   94   4    3    1.0000     0.02500   -1
```

IN.OCC

```
1 1 1 1 1 1 1 1 1 1

1 1 1 0.66666666666666

0.66666666666666 0.66666666666666 1
```

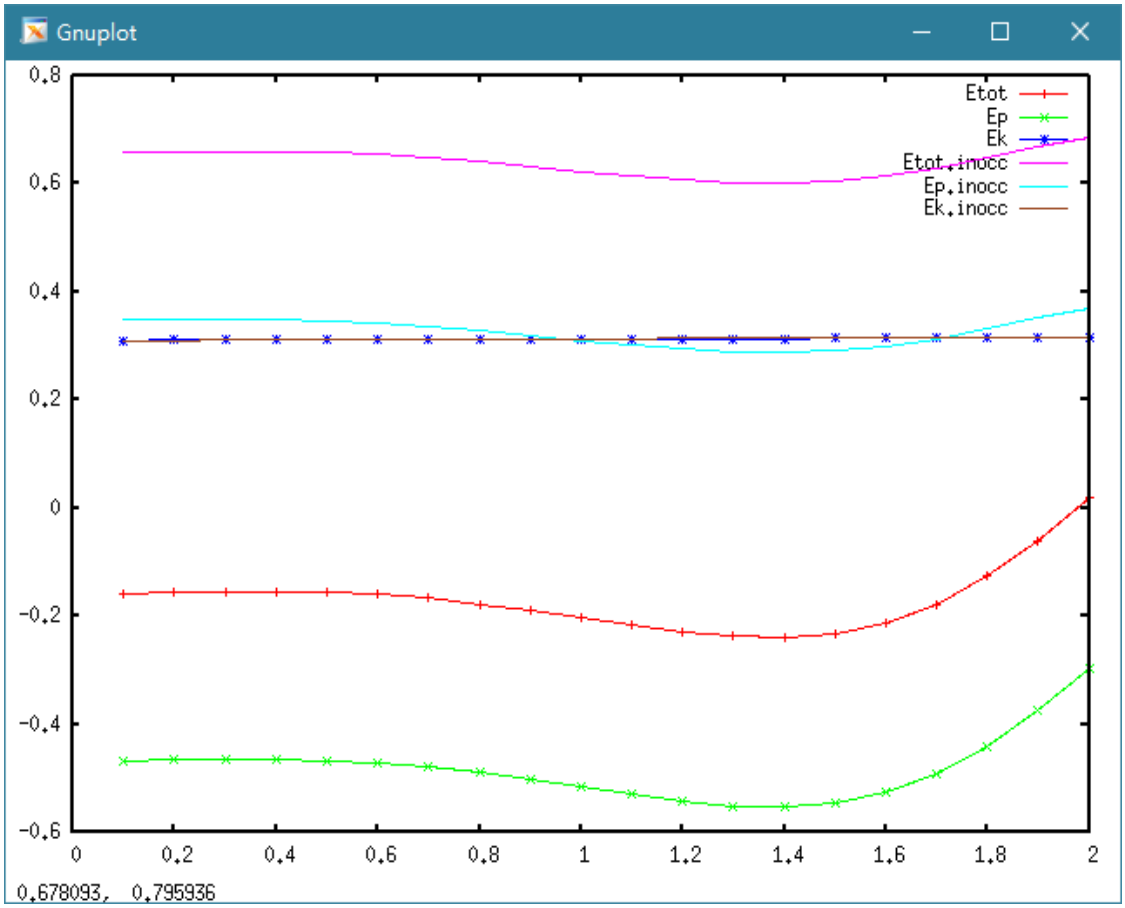
```
0 0 0 0 0 0 0 0 0 0 0 0 0
```

IN.CC

```
1  1 1.0

1  2 1.0

1  3 1.0

1  4 1.0

1  5 1.0

1  6 1.0

1  7 1.0

1  8 1.0

1  9 1.0

1  10 1.0

1  11 1.0

1  12 1.0

1  13 1.0

1  14 1.0

1  15 1.0

2  16 0.8  17 0.2

1  17 1.0

1  18 1.0

1  19 1.0

1  20 1.0

1  21 1.0

1  22 1.0

1  23 1.0

1  24 1.0
```

```
1  25 1.0

1  26 1.0

1  27 1.0

1  28 1.0

1  29 1.0

1  30 1.0
```

Etot,Ep,Ek plot:



9.MD_DETAIL = MD, MSTEP, DT, TEMP1, TEMP2

default: no default setting.

description:

Note: this is a required line for JOB=MD and JOB=TDDFT. (ref. PWmat manual 2.1.6.)

10.TDDFT_STIME=stime

description:

stime used for restart TDDFT, is the starting time of TDDFT. fs unit.

see RESTART.

11.RESTART

description:

needed settings:

MD_DETAIL=11,...

IN.RHO=T

IN.WG=T

TDDFT_STIME=stime

needed files:

		IN.ATOM=atom.config from MOVEMENT
spin	1,22	OUT.WG-->IN.WG OUT.RHO-->IN.RHO OUT.TDDFT-->IN.TDDFT
	2	OUT.WG-->IN.WG OUT.RHO-->IN.RHO OUT.TDDFT-->IN.TDDFT OUT.WG_2-- >IN.WG_2 OUT.RHO_2-->IN.RHO_2 OUT.TDDFT-->IN.TDDFT
	222	OUT.WG-->IN.WG OUT.RHO-->IN.RHO OUT.RHO_SOM-->IN.RHO_SOM OUT.TDDFT-- >IN.TDDFT

example4:

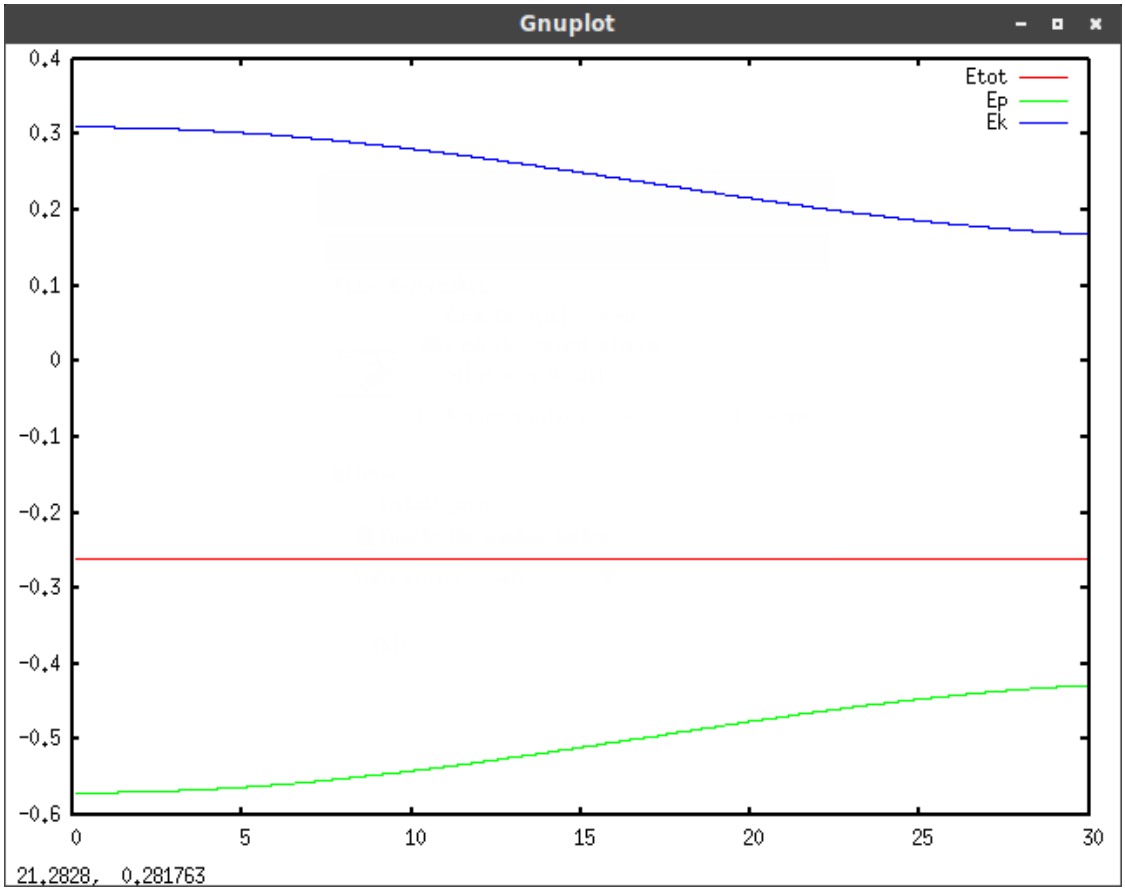
One TDDFT. killed at 329 step.

```
    1        1

IN.ATOM   = atom.config

JOB       = TDDFT

MD_DETAIL = 1, 1000, 0.1, 300,300

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF

Ecut      =   30

N123      =   32   32   32

OUT.TDDFT = T T 100 T  100
```

Files we get:

OUT.WG,OUT.RHO,OUT.TDDFT	of step 300
MOVEMENT,MDSTEPS	each step

Etot,Ep,Ek plot:



Resart TDDFT from step 300.

```
1         1

IN.ATOM   = atom.config.300

JOB       = TDDFT

MD_DETAIL = 11, 1000, 0.1, 300,300

TDDFT_STIME = 30.10

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF

Ecut      =    30

N123      =    32    32    32

IN.WG     = T

IN.RHO    = T
```

get **atom.config.300** from MOVEMENT:

```
  8 atoms,Iteration=  300, Etot,Ep,Ek=   -0.9342598856E+03  -0.9344282212E+03
0.6186218552E-02
```

Lattice vector

0.5650000000E+01 0.0000000000E+00 0.0000000000E+00

0.0000000000E+00 0.5650000000E+01 0.0000000000E+00

0.0000000000E+00 0.0000000000E+00 0.5650000000E+01

Position, move_x, move_y, move_z

31 -0.002650892 -0.001549781 0.011701363 1 1 1

31 -0.001826470 0.515825032 0.496601858 1 1 1

31 0.488596782 -0.003825035 0.504426022 1 1 1

31 0.512901546 0.489831560 0.011845858 1 1 1

33 0.239192635 0.257254096 0.240225612 1 1 1

33 -0.259114091 -0.256079157 0.251123637 1 1 1

33 -0.236278788 0.244572796 -0.256805443 1 1 1

33 0.259907060 -0.245082351 -0.255548664 1 1 1

Force

31 -0.096760713 0.083896371 0.811411472

31 -0.306358278 0.454455044 -0.165768770

31 -0.457764036 -0.668564451 0.440678002

31 0.270932363 0.190182527 1.051391132

33 0.145648837 -0.242459725 -0.535882141

33 0.320371309 -0.343051872 -0.525941728

33 -0.006120575 0.196394131 -0.248770888

33 0.133291806 0.338118523 -0.829419823

Velocity

31 -0.001058344 -0.000666545 0.001646305

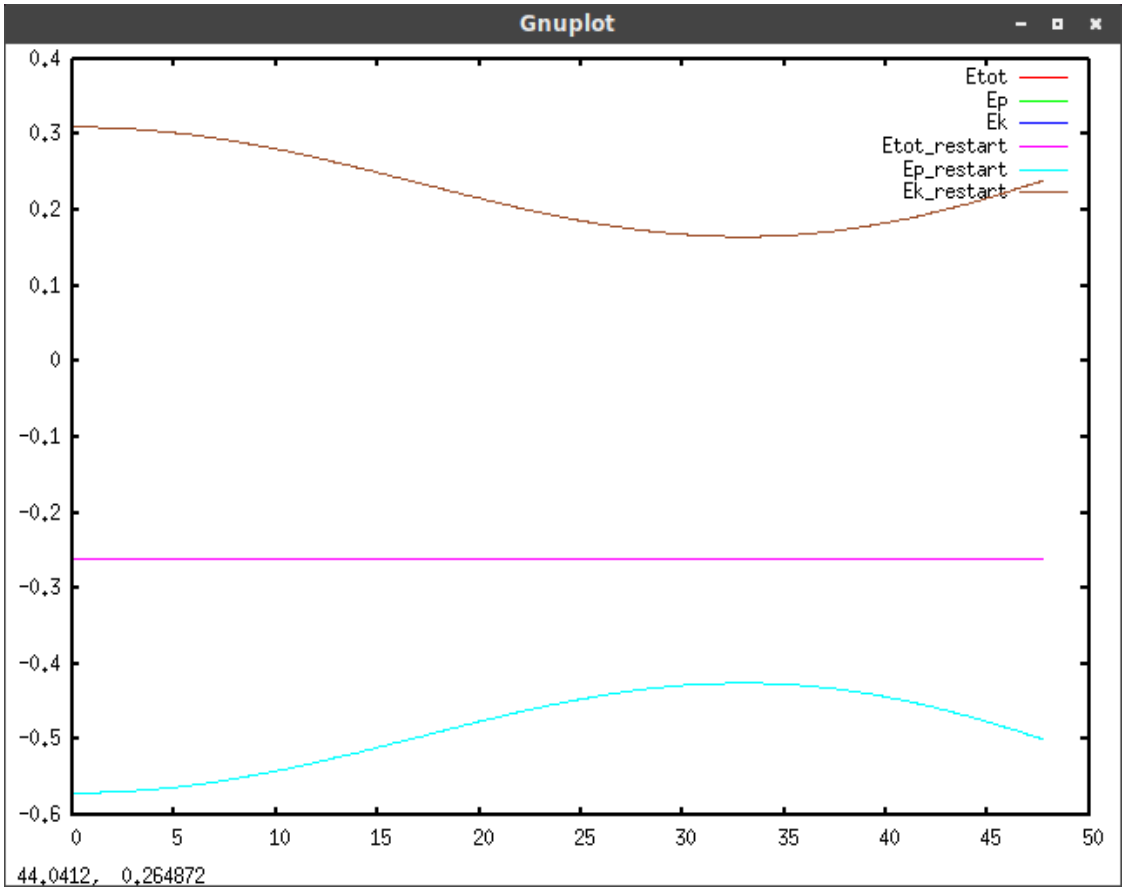
31 0.000164137 0.003853948 -0.001632847

```
 31   -0.002791301    0.000563892    0.000291948

 31    0.003814745   -0.004180976    0.001003179

 33   -0.004180128    0.003104497   -0.001841969

 33   -0.004002909   -0.001311052    0.001932642

 33    0.004825449   -0.002372473   -0.001588050

 33    0.003241180    0.000975878    0.000279484
```

get IN.RHO IN.WG IN.TDDFT

```
cp OUT.RHO IN.RHO

cp OUT.WG IN.WG

cp OUT.TDDFT IN.TDDFT
```

Etot,Ep,Ek plot:



example:

restart with external potential.

13.SHOW_RESULTS

OUT.TDDFT---plot_tddft.f
TDDOS---DOS
MDDIPOLE.RSPACE

14.影响稳定性的因素（参数调节）

accuracy & precision.

example5:

etot.input.lowprec

```
1          1

IN.ATOM   = atom.config

JOB       = TDDFT

MD_DETAIL = 1, 20, 0.1, 300,300

TDDFT_DETAIL = 1,30,30

XCFUNCTIONAL = PBE

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF

Ecut      =   30.0

num_band  =  30

N123      = 32 32 32
```

MDSTEPS.lowprec

```
Iter=  0.100000E+00 Etot,Ep,Ek=   -0.9362093590E+03  ..... Fcheck= -.120E+01

Iter=  0.200000E+00 Etot,Ep,Ek=   -0.9362093489E+03  ..... Fcheck= 0.704E+00

Iter=  0.300000E+00 Etot,Ep,Ek=   -0.9362093460E+03  ..... Fcheck= 0.911E+00

Iter=  0.400000E+00 Etot,Ep,Ek=   -0.9362093497E+03  ..... Fcheck= 0.111E+01

Iter=  0.500000E+00 Etot,Ep,Ek=   -0.9362093568E+03  ..... Fcheck= 0.119E+01

Iter=  0.600000E+00 Etot,Ep,Ek=   -0.9362093388E+03  ..... Fcheck= 0.717E+00

Iter=  0.700000E+00 Etot,Ep,Ek=   -0.9362093419E+03  ..... Fcheck= 0.107E+01
```

```
Iter=  0.800000E+00 Etot,Ep,Ek=   -0.9362093367E+03  ..... Fcheck= 0.920E+00

Iter=  0.900000E+00 Etot,Ep,Ek=   -0.9362093433E+03  ..... Fcheck= 0.111E+01

Iter=  0.100000E+01 Etot,Ep,Ek=   -0.9362093398E+03  ..... Fcheck= 0.955E+00

Iter=  0.110000E+01 Etot,Ep,Ek=   -0.9362093479E+03  ..... Fcheck= 0.111E+01

Iter=  0.120000E+01 Etot,Ep,Ek=   -0.9362093371E+03  ..... Fcheck= 0.888E+00

Iter=  0.130000E+01 Etot,Ep,Ek=   -0.9362093286E+03  ..... Fcheck= 0.913E+00

Iter=  0.140000E+01 Etot,Ep,Ek=   -0.9362093363E+03  ..... Fcheck= 0.109E+01

Iter=  0.150000E+01 Etot,Ep,Ek=   -0.9362093373E+03  ..... Fcheck= 0.101E+01

Iter=  0.160000E+01 Etot,Ep,Ek=   -0.9362093391E+03  ..... Fcheck= 0.102E+01

Iter=  0.170000E+01 Etot,Ep,Ek=   -0.9362093416E+03  ..... Fcheck= 0.103E+01

Iter=  0.180000E+01 Etot,Ep,Ek=   -0.9362093388E+03  ..... Fcheck= 0.974E+00

Iter=  0.190000E+01 Etot,Ep,Ek=   -0.9362093428E+03  ..... Fcheck= 0.104E+01

Iter=  0.200000E+01 Etot,Ep,Ek=   -0.9362093324E+03  ..... Fcheck= 0.921E+00
```

etot.input.highprec

```
1          1

IN.ATOM   = atom.config

JOB       = TDDFT

convergence=difficult

precision=double

MD_DETAIL = 1, 20, 0.1, 300,300

TDDFT_DETAIL = 1,30,30

XCFUNCTIONAL = PBE

IN.PSP1   = 31-Ga.LDA.fhi.UPF

IN.PSP2   = 33-As.LDA.fhi.UPF

Ecut      =   30.0

num_band  =  30
```

```
 N123     = 32 32 32
```

MDSTEPS.highprec

```
 Iter=  0.100000E+00 Etot,Ep,Ek=   -0.9362093469E+03 .... Fcheck= 0.123E+00

 Iter=  0.200000E+00 Etot,Ep,Ek=   -0.9362093463E+03 .... Fcheck= 0.977E+00

 Iter=  0.300000E+00 Etot,Ep,Ek=   -0.9362093462E+03 .... Fcheck= 0.996E+00

 Iter=  0.400000E+00 Etot,Ep,Ek=   -0.9362093459E+03 .... Fcheck= 0.993E+00

 Iter=  0.500000E+00 Etot,Ep,Ek=   -0.9362093456E+03 .... Fcheck= 0.993E+00

 Iter=  0.600000E+00 Etot,Ep,Ek=   -0.9362093456E+03 .... Fcheck= 0.100E+01

 Iter=  0.700000E+00 Etot,Ep,Ek=   -0.9362093457E+03 .... Fcheck= 0.100E+01

 Iter=  0.800000E+00 Etot,Ep,Ek=   -0.9362093456E+03 .... Fcheck= 0.998E+00

 Iter=  0.900000E+00 Etot,Ep,Ek=   -0.9362093457E+03 .... Fcheck= 0.100E+01

 Iter=  0.100000E+01 Etot,Ep,Ek=   -0.9362093454E+03 .... Fcheck= 0.996E+00

 Iter=  0.110000E+01 Etot,Ep,Ek=   -0.9362093450E+03 .... Fcheck= 0.995E+00

 Iter=  0.120000E+01 Etot,Ep,Ek=   -0.9362093446E+03 .... Fcheck= 0.995E+00

 Iter=  0.130000E+01 Etot,Ep,Ek=   -0.9362093442E+03 .... Fcheck= 0.995E+00

 Iter=  0.140000E+01 Etot,Ep,Ek=   -0.9362093440E+03 .... Fcheck= 0.998E+00

 Iter=  0.150000E+01 Etot,Ep,Ek=   -0.9362093439E+03 .... Fcheck= 0.999E+00

 Iter=  0.160000E+01 Etot,Ep,Ek=   -0.9362093438E+03 .... Fcheck= 0.999E+00

 Iter=  0.170000E+01 Etot,Ep,Ek=   -0.9362093439E+03 .... Fcheck= 0.100E+01

 Iter=  0.180000E+01 Etot,Ep,Ek=   -0.9362093438E+03 .... Fcheck= 0.999E+00

 Iter=  0.190000E+01 Etot,Ep,Ek=   -0.9362093440E+03 .... Fcheck= 0.100E+01

 Iter=  0.200000E+01 Etot,Ep,Ek=   -0.9362093440E+03 .... Fcheck= 0.100E+01
```

dt.

example:

etot.input.lowprec & small dt.

system size.

example:

integration accuracy.

example

others sys_type, in.ferup-->in.occ,