How to use HVT's linear response method function

First, the user can invoke the linear response method calculation function of HVT by “hvt -linearU”. Note: This function of HVT needs to be used in conjunction with VASP, and is only applicable to VASP calculations.

```
hb@LAPTOP:~/case1$ hvt -linearU
*** Script for Linear response calculation of U ***
⟶ Select the calculation you want to perform:
    0.Instructions;
    1.Input example;
    2.DFT groudstate;
    3.SCF and NSCF for DFT+U(After 2);
    4.Submit all calculations(After 3);
    5.Extract Ueff data(After 3).
    6.Linear fitting of the potential and the number of electrons (drawing)
⟶
```

The “hvt -linearU” menu screen has seven functions, of which function 0 is the instructions for use, function 1 is the input file case, function 2 is the base state calculation, function 3 is the self-adjoint and non-self-adjoint DFT+U calculation, function 4 is the batch task submission function, function 5 is the calculation of U-values, and function 6 is the plotting.

```
hb@LAPTOP:~/case1$ hvt -linearU
*** Script for Linear response calculation of U ***
⟶ Select the calculation you want to perform:
    0.Instructions;
    1.Input example;
    2.DFT groudstate;
    3.SCF and NSCF for DFT+U(After 2);
    4.Submit all calculations(After 3);
    5.Extract Ueff data(After 3).
    6.Linear fitting of the potential and the number of electrons (drawing)
⟶ 0
⟶
1). Create a new folder and prepare the calculation file;
2). Write the commit command script inside the sub.sh
3). Input file cases can be generated using function 1;
4). Run the function after preparing the input file 2;
5). Considering the different server environments,
    this function does not provide a batch submission function;
6). First go to the 1-DFT folder to check and submit calculations;
7). Then run function 3 and go to the 2-NCSF+SCF folder to check and submit all the tasks;
8). After the above calculations are completed run function 4 to calculate and output the results;
9). The output file is Udata.log and its last line is the calculated U value;
10). Access to special folders command: cd -- -0.20;
11). Add -- to all operations on folders named -0.XX, e.g. 10);
12). tebiezhu Special note: It is recommended that calculations be performed with protocells.
```

```
hb@LAPTOP:~/case1$ hvt -linearU
*** Script for Linear response calculation of U ***
--> Select the calculation you want to perform:
    0.Instructions;
    1.Input example;
    2.DFT groudstate;
    3.SCF and NSCF for DFT+U(After 2);
    4.Submit all calculations(After 3);
    5.Extract Ueff data(After 3).
    6.Linear fitting of the potential and the number of electrons (drawing)
--> 1
--> Please enter the input file you want to generate:
    1.INCAR(Incomplete)
    2.KPOINTS
    3.POTCAR
-->
```

Functions 2, 3, 5, and 6 of "hvt -linearU" are the core of this function, where function 2 creates the computation folder and prepares the input files for the base state computation.

Special note: For antiferromagnetic systems, the user needs to pay extra attention to the setting of the "MAGMOM" label.

To use Function 2 you need to follow the prompts to select Plus U Element and Plus U Track.

```
hb@LAPTOP:~/case1$ ls
INCAR  KPOINTS  POSCAR  POTCAR
hb@LAPTOP:~/case1$ hvt -linearU
*** Script for Linear response calculation of U ***
--> Select the calculation you want to perform:
    0.Instructions;
    1.Input example;
    2.DFT groudstate;
    3.SCF and NSCF for DFT+U(After 2);
    4.Submit all calculations(After 3);
    5.Extract Ueff data(After 3).
    6.Linear fitting of the potential and the number of electrons (drawing)
--> 2
--> Select the element by number to calculate the U value( 1-Fe 2-O ):
--> 1
--> Number of the orbital you want to calculate the U value:1-p;2-d;3-f
--> 2
--> Finish.
```

After using "hvt -linearU", look at the folder, you will find that HVT has created two new folders, "1-DFT" is the folder used to calculate the ground state, "2-NCSF

+SCF" is for calculating self-consistent and non-self-consistent DFT+U.

```
hb@LAPTOP:~/case1$ ls
1-DFT  2-NCSF+SCF  INCAR  KPOINTS  POSCAR  POSCAR.0  POTCAR  input.log
hb@LAPTOP:~/case1$ ls 1-DFT/ 2-NCSF+SCF/
1-DFT/:
INCAR  KPOINTS  POSCAR  POTCAR

2-NCSF+SCF/:
-0.05  -0.10  -0.15  -0.20  0.00  0.05  0.10  0.15  0.20
```

Next, you need to go to the "1-DFT" folder to check the input file and submit the calculation.

```
hb@LAPTOP:~/case1$ cd 1-DFT/
hb@LAPTOP:~/case1$ ls
INCAR  KPOINTS  POSCAR  POTCAR
hb@LAPTOP:~/case1$ nohup mpirun -np 40 vasp_std&
```

After the calculation is completed, go back to the previous folder and run function 3 of "hvt -linearU". HVT will prepare the input files for self-consistent and non-self-consistent calculations in the "2-NCSF+SCF" folder based on the results of the ground state calculations files in the "2-NCSF+SCF" folder.

```
hb@LAPTOP:~/case1$ ls
CHG  CHGCAR  CONTCAR  DOSCAR  EIGENVAL  IBZKPT  INCAR  KPOINTS  OSZICAR  OUTCAR
PCDAT  POSCAR  POTCAR  PROCAR  REPORT  WAVECAR  XDATCAR  out.log  vasprun.xml
hb@LAPTOP:~/case1$ cd ..
hb@LAPTOP:~/case1$ ls
1-DFT  2-NCSF+SCF  INCAR  KPOINTS  POSCAR  POSCAR.0  POTCAR  input.log
hb@LAPTOP:~/case1$ hvt -linearU
*** Script for Linear response calculation of U ***
--> Select the calculation you want to perform:
    0.Instructions;
    1.Input example;
    2.DFT groudstate;
    3.SCF and NSCF for DFT+U(After 2);
    4.Submit all calculations(After 3);
    5.Extract Ueff data(After 3).
    6.Linear fitting of the potential and the number of electrons (drawing)
--> 3
--> Finish.
```

Function 4 of “hvt -linearU” is a function to batch submit self-consistent and non-self-consistent computation tasks. Before using this function, you need to prepare a batch in all the innermost subfolders of “2-NCSF+SCF”. Before using this function, you need to prepare a “sub.sh” file and the user's own submission script in all the innermost subfolders of “2-NCSF+SCF”, and the following is an example of the “sub.sh” script:

1. If the user's own submission script is a PBS queue submission script: “submission.pbs”:

```
#!/bin/bash
qsub submission.pbs
```

2. If the user's own submission script is a SLURM queue submission script: “submission.batch”:

```
#!/bin/bash
sbatch submission.batch
```

3. If the user is using “nohup mpirun -np 40 vasp_std&” to submit VASP calculations:

```
#!/bin/bash
nohup mpirun -np 40 vasp_std&
```

Note: Due to the need to check the input file before calculating, and the possible limitations of the user's computational resources, it is not recommended to submit batch calculations using the “hvt -linearU” function4 unless the user is very confident in the completeness of his/her file and has sufficient computational resources.

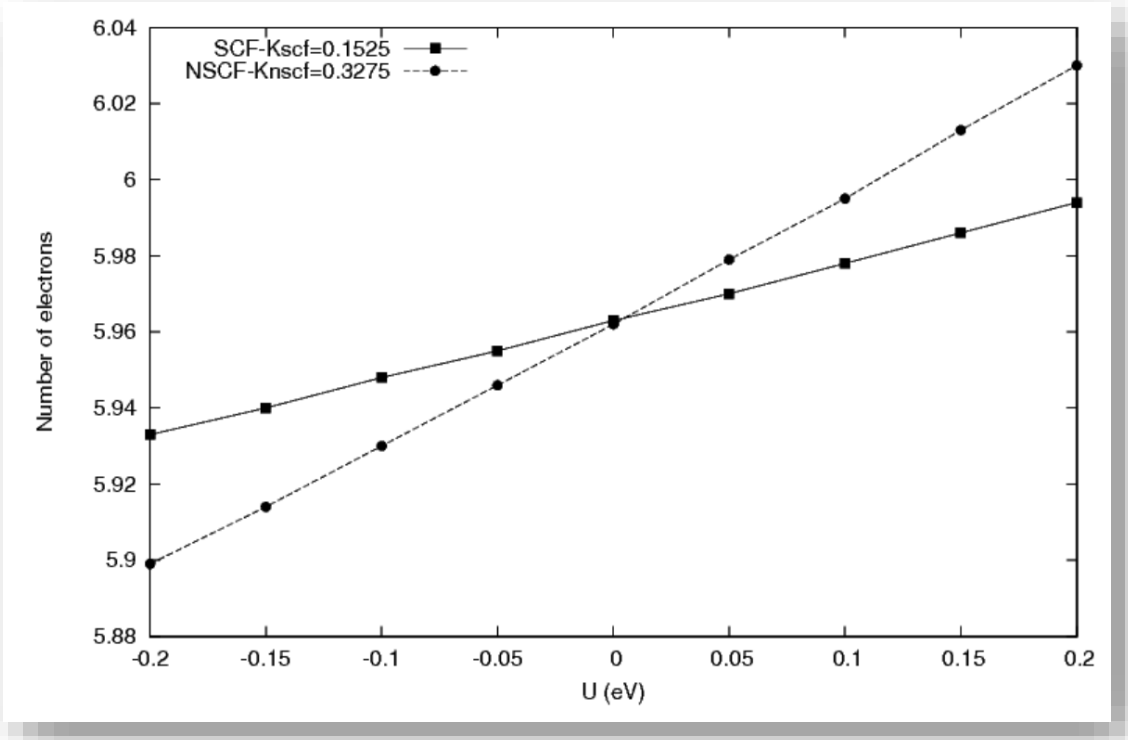
After the above calculations are done, the user needs to calculate the U-value using the function 5 of “hvt -linearU”.

```
hb@LAPTOP:~/case1$ ls
1-DFT  2-NCSF+SCF  INCAR  KPOINTS  POSCAR  POSCAR.0  POTCAR  input.log
hb@LAPTOP:~/case1$ hvt -linearU
*** Script for Linear response calculation of U ***
──> Select the calculation you want to perform:
    0.Instructions;
    1.Input example;
    2.DFT groudstate;
    3.SCF and NSCF for DFT+U(After 2);
    4.Submit all calculations(After 3);
    5.Extract Ueff data(After 3).
    6.Linear fitting of the potential and the number of electrons (drawing)
──> 5
──>
*** Select information ***
+═══════════════════════════════+
|  Element  cal_num  atom_num |
├───────────────────────────────┤
|       Fe        1        12 |
+═══════════════════════════════+

*** Data ***
U       DFT      NSCF     SCF
─────   ─────    ─────    ─────
-0.20    5.963    5.899    5.933
-0.15    5.963    5.914    5.940
-0.10    5.963    5.930    5.948
-0.05    5.963    5.946    5.955
0.00    5.963    5.962    5.963
0.05    5.963    5.979    5.970
0.10    5.963    5.995    5.978
0.15    5.963    6.013    5.986
0.20    5.963    6.030    5.994
─────   ─────    ─────    ─────

*** Results: ***
Ueff:  3.50394
```

Once the calculation is complete, you can use the “hvt -linearU” function6 to get the relationship between the change in the number of d-electrons of the select atoms in crystal and the value of U.



The examples used in this note are in “linear U examples.zip”.