Dynamical Mean Field Theory for strongly correlated electrons

TOOLbox series, nov 2021

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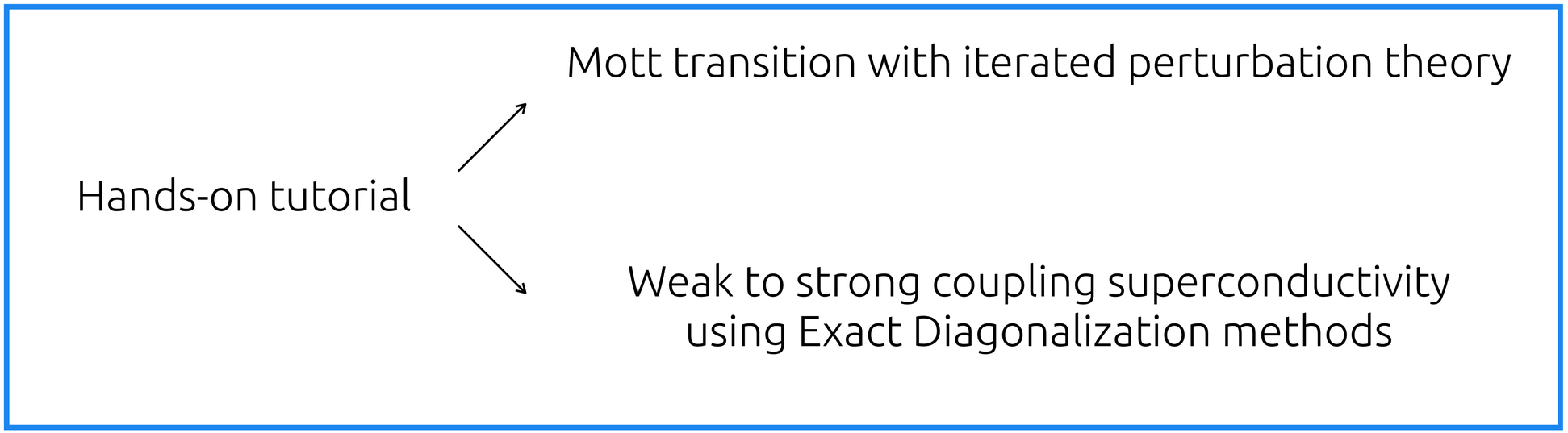
DQMP, Unige

Monday 22

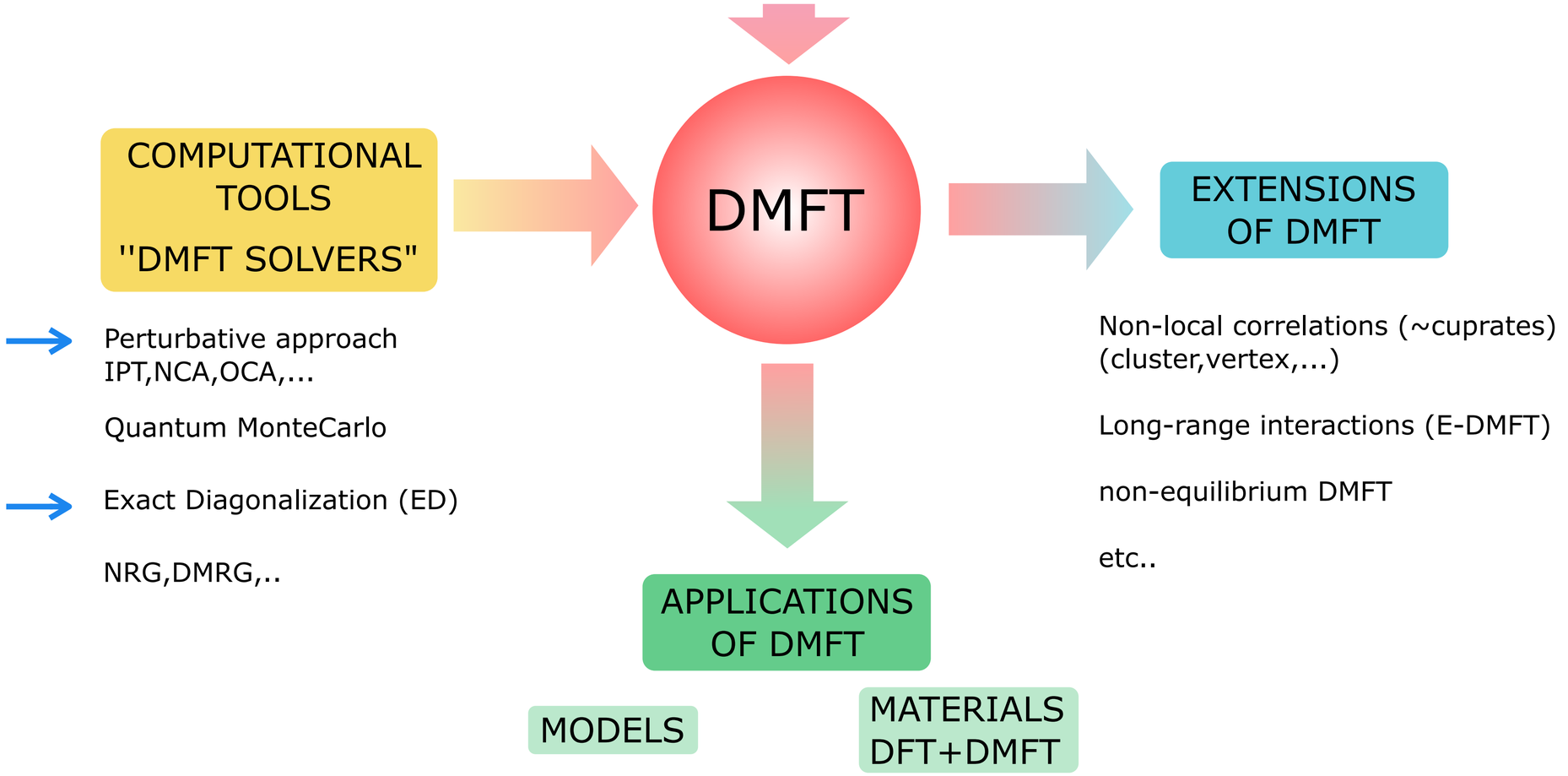
Introduction to the basics concepts of the Dynamical Mean Field Theory

(instruction for the hands-on tutorial)

Tuesday 23



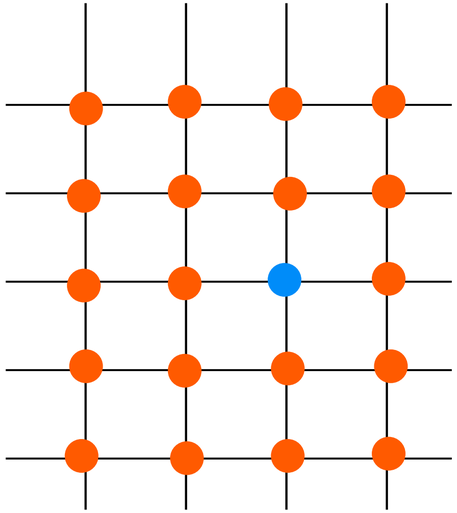
General concepts of statistic physics
(single site representation, limit of infinite dimensions,..)



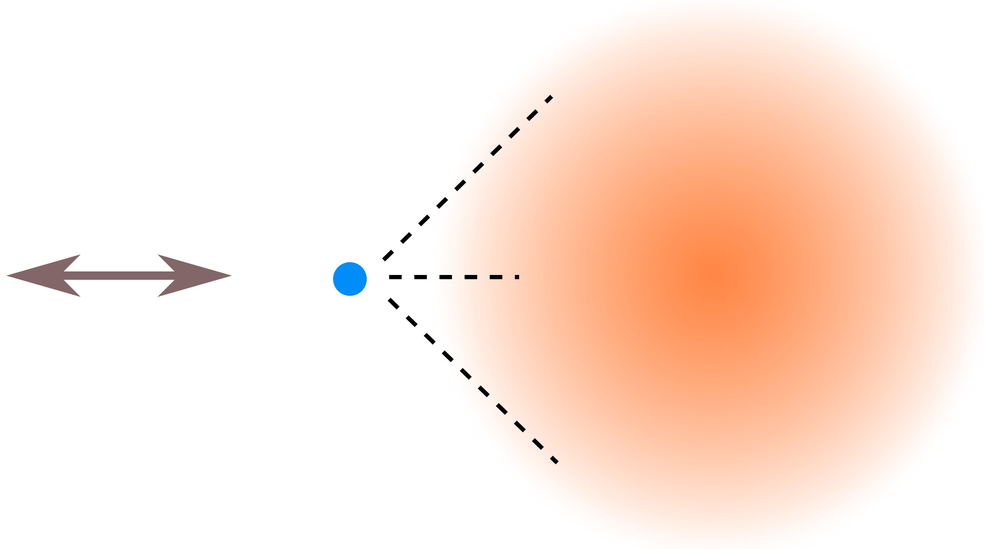
Adapted from A. Georges
Fermions en interaction: Introduction a la theorie du champ moyen dynamique. College de France, 2019 (online)

$$H_{\text{Hubbard}} = -t \sum_{\langle \mathbf{R}\mathbf{R}' \rangle \sigma} c^{\dagger}_{\mathbf{R}\sigma} c_{\mathbf{R}'\sigma} + U \sum_{\mathbf{R}} n_{\mathbf{R}\uparrow} n_{\mathbf{R}\downarrow} - \mu \sum_{\mathbf{R}\sigma} c^{\dagger}_{\mathbf{R}\sigma} c_{\mathbf{R}\sigma},$$

Lattice problem



Single-site representation



Compare with static mean-field

$$H_{\text{Ising}} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - \sum_i h_i \sigma_i$$

	STATIC MeanField	DYNAMICAL MeanField
LOCAL OBSERVABLE	local magnetization $m_i = \langle \sigma_i \rangle$	local Greens function $G_{ii}(\tau) = -\langle T_\tau c_{i\sigma}(\tau) c^\dagger_{i\sigma}(0) \rangle$
LOCAL REPRESENTATION	spin in a magnetic field $m_i = \tanh\left(\beta h_i^{\text{eff}}\right)$	atom in a bath $G^{-1}_{ii}(\tau) = \mathcal{G}_0^{-1}(\tau) - \Sigma_{\text{imp}}[\mathcal{G}_0]$
SELF CONSISTENCY RELATION	$h_i^{\text{eff}} = h_i + J \sum_{\langle ij \rangle} m_j$	$\Sigma_{\mathbf{k}}(\omega) = \Sigma_{imp}(\omega)$

$$\mathcal{S}^{(i)}_{\rm imp} = \int d\tau d\tau' c^\dagger_{i\sigma} \mathcal{G}_0^{-1}(\tau-\tau') c_{i\sigma}(\tau') + \int d\tau H^{(i)}_{int}(\tau) \qquad H^{(i)}_{int} = U n_{i\uparrow} n_{i\downarrow}$$

$$\mathcal{G}_0^{-1}(\tau-\tau') = G^{-1}_{at,0}(\tau-\tau') - \Delta(\tau-\tau'). \qquad G_{at,0}(i\omega_n) = i\omega_n + \mu$$

$$G_{ii,\sigma}(\tau-\tau') = -\langle T_\tau c_{i\sigma}(\tau) c^\dagger_{i\sigma}(\tau') \rangle_{\mathrm{imp}[\mathcal{G}_0]}$$

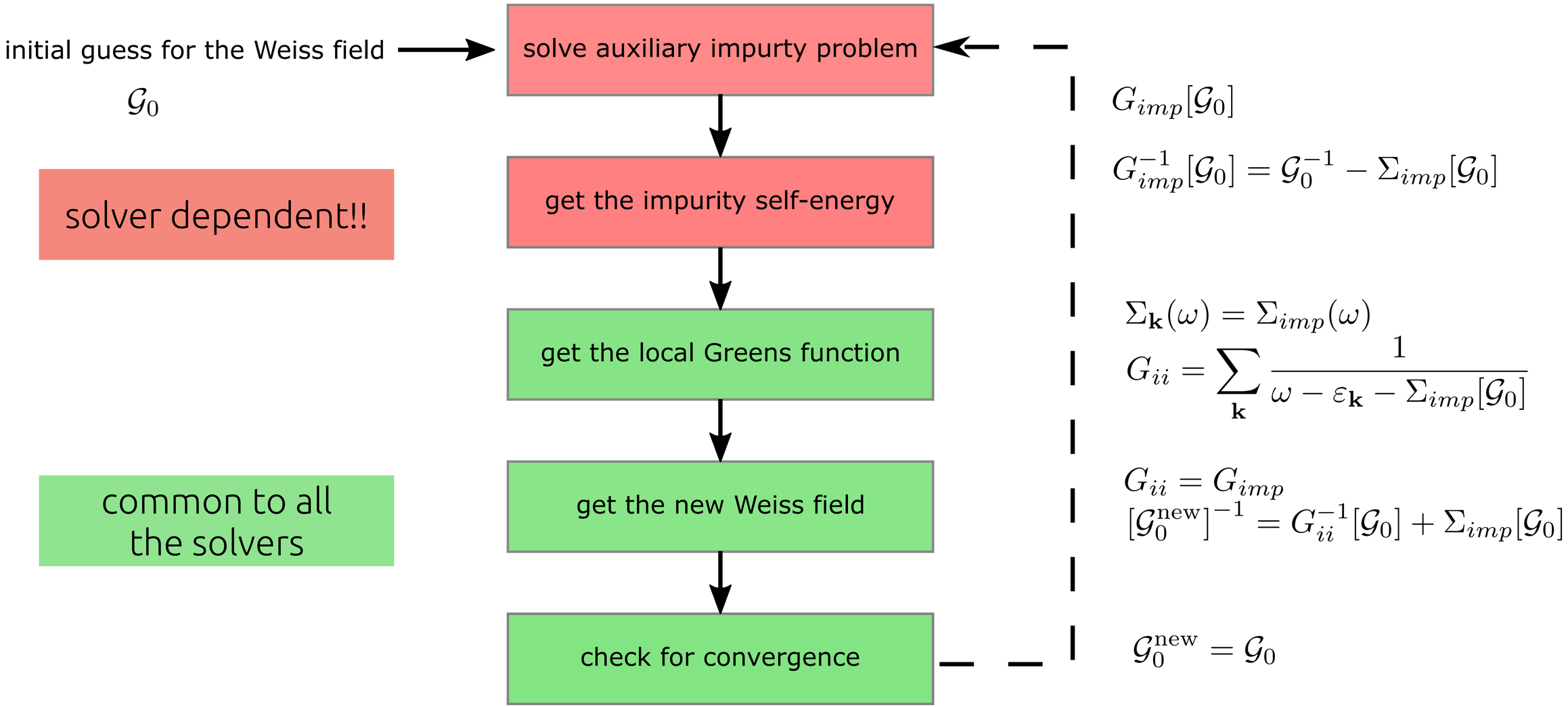
$$G^{-1}_{ii\sigma}(\tau-\tau') = \mathcal{G}_0^{-1}(\tau-\tau') - \Sigma_{\rm imp}[\mathcal{G}_0]$$

DMFT approximation

$$\boxed{\Sigma_{\mathbf{k}} = \Sigma_{\rm imp}[\mathcal{G}_0]}$$

exact for $z \to \infty$

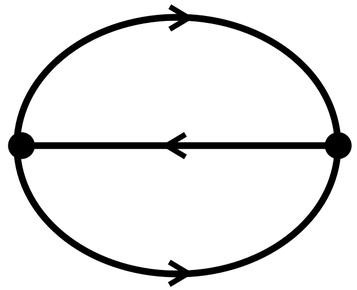
$$G_{ii}(\omega) = \sum_{\mathbf{k}} \frac{1}{\omega - \varepsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}(\omega)}$$


initial guess for the Weiss field
$\mathcal{G}_0$
solver dependent!!
common to all the solvers
solve auxiliary impurty problem
get the impurity self-energy
get the local Greens function
get the new Weiss field
check for convergence
$G_{imp}[\mathcal{G}_0]$
$G^{-1}_{imp}[\mathcal{G}_0] = \mathcal{G}_0^{-1} - \Sigma_{imp}[\mathcal{G}_0]$
$\Sigma_{\mathbf{k}}(\omega) = \Sigma_{imp}(\omega)$
$G_{ii} = \sum_{\mathbf{k}} \frac{1}{\omega - \varepsilon_{\mathbf{k}} - \Sigma_{imp}[\mathcal{G}_0]}$
$G_{ii} = G_{imp}$
$[\mathcal{G}_0^{\rm new}]^{-1} = G^{-1}_{ii}[\mathcal{G}_0] + \Sigma_{imp}[\mathcal{G}_0]$
$\mathcal{G}_0^{\rm new} = \mathcal{G}_0$

Iterated Perturbation Theory (IPT)

Approximate solution of the impurity problem

$$\Sigma_{\mathrm{imp}}(\tau) = U^2 \mathcal{G}_0(\tau)\mathcal{G}_0(-\tau)\mathcal{G}_0(\tau)$$

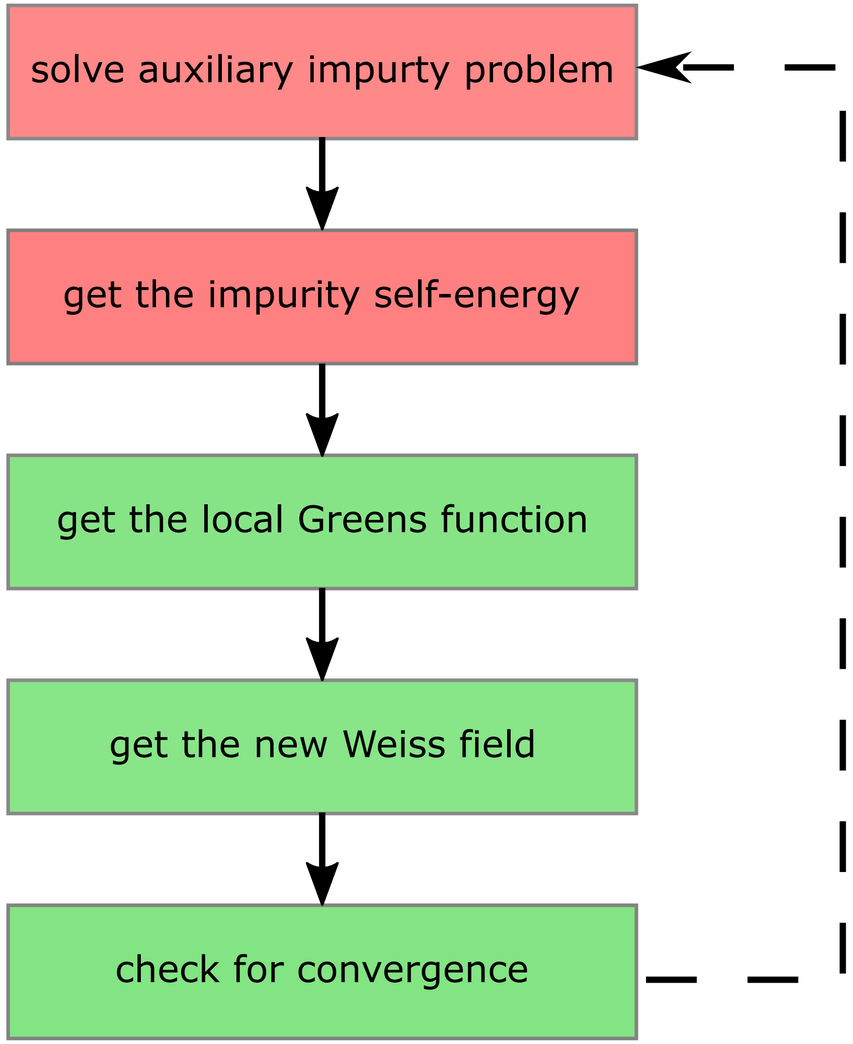


- Mott transition in the single-band Hubbard model
- Useful to get used with the DMFT loop
- Imaginary frequency or real frequency
- Little practical use beyond the single-band Hubbard model

ipt_hm_matsubara.f90

wm(:) !Matsubara frequencies
Sigma(:) !impurity Self-energy
fg0(:) !Weiss field at loop iloop
fg0_prev(:) !Weiss field at loop iloop-1
fg(:) !local greens function

```
!get or read first sigma
call  get_initial_function(Sigma,"Sigma.restart")
!dmft loop:
iloop=0 ; converged=.false.
do while(.not.converged.AND.iloop<nloop)
   iloop=iloop+1
   write(*,"(A,i5)",advance="no")"DMFT-loop",iloop
   !SELF-CONSISTENCY:
   do i=1,L
      zeta  = xi*wm(i) - sigma(i)
      fg(i) = gfbethe(wm(i),zeta,D)
   enddo
   !
   fg0_prev= fg0                        !
   fg0     = one/(one/fg + sigma)
   if(iloop>1)fg0 = wmix*fg0 + (1.d0-wmix)*fg0_prev !mix to avoid loops
   !
   !IMPURITY SOLVER: fg0-->sigma
   call solve_ipt_mats(sigma)
   !
   dens = ipt_measure_dens_matsubara(fg)
   z    = ipt_measure_zeta_matsubara(sigma,fg0)
   docc = ipt_measure_docc_matsubara(sigma,fg0)
   write(*,"(3F15.9,3x)",advance="no")dens,docc,z
   !Check CONVERGENCE on the Weiss Field:
   converged=check_convergence(fg0)
enddo
```



ipt_hm_matsubara.f90

```
wm(:)        !Matsubara frequencies
Sigma(:)     !impurity Self-energy
fg0(:)       !Weiss field at loop iloop
fg0_prev(:)  !Weiss field at loop iloop-1
fg(:)        !local greens function
```

Initialise the loop

```
!get or read first sigma
call  get_initial_function(Sigma,"Sigma.restart")
!dmft loop:
iloop=0 ; converged=.false.
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   iloop=iloop+1
   write(*,"(A,i5)",advance="no")"DMFT-loop",iloop
   !SELF-CONSISTENCY:
   do i=1,L
      zeta  = xi*wm(i) - sigma(i)
      fg(i) = gfbethe(wm(i),zeta,D)
   enddo
   !
   fg0_prev= fg0                        !
   fg0     = one/(one/fg + sigma)
   if(iloop>1)fg0 = wmix*fg0 + (1.d0-wmix)*fg0_prev !mix to avoid loops
   !
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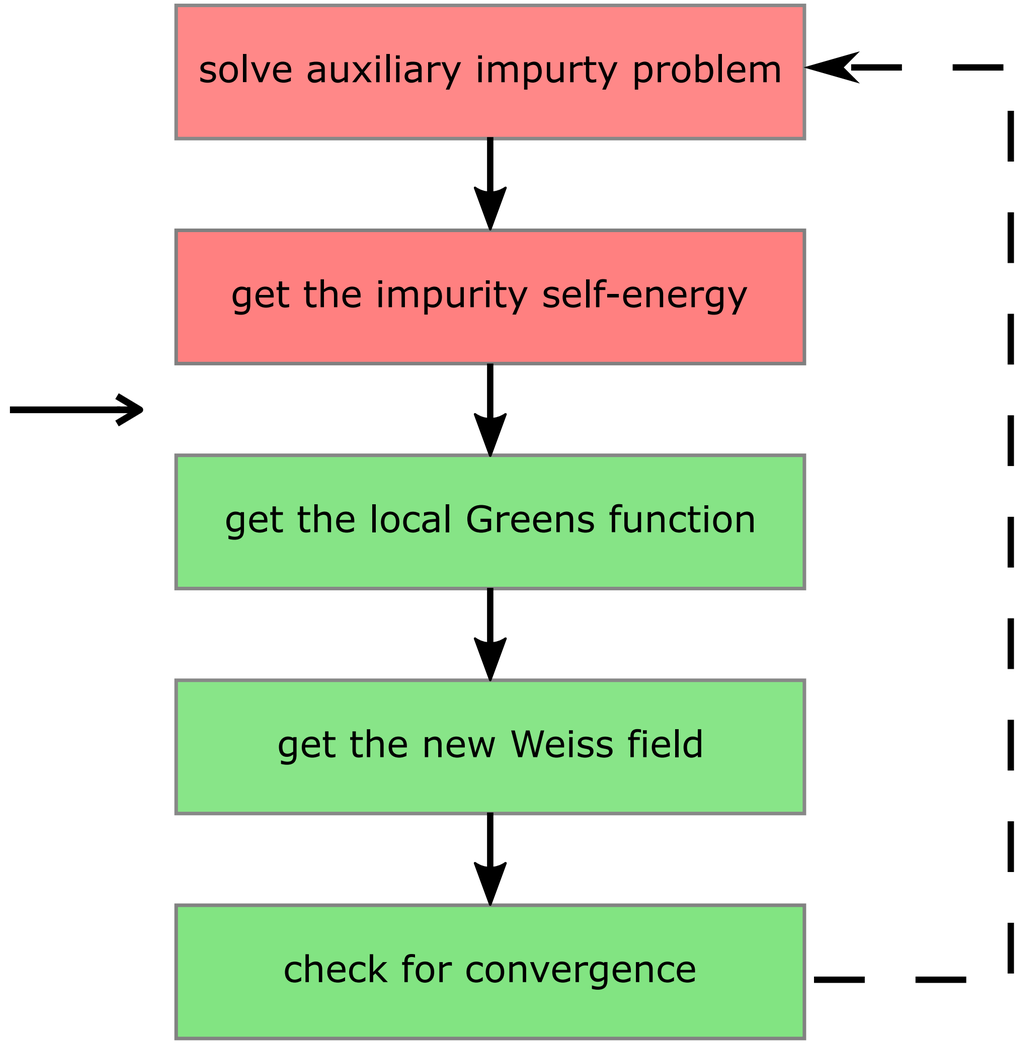

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   !SELF-CONSISTENCY:
   do i=1,L
      zeta  = xi*wm(i) - sigma(i)
      fg(i) = gfbethe(wm(i),zeta,D)
   enddo
   !
   fg0_prev= fg0                          !
   fg0     = one/(one/fg + sigma)
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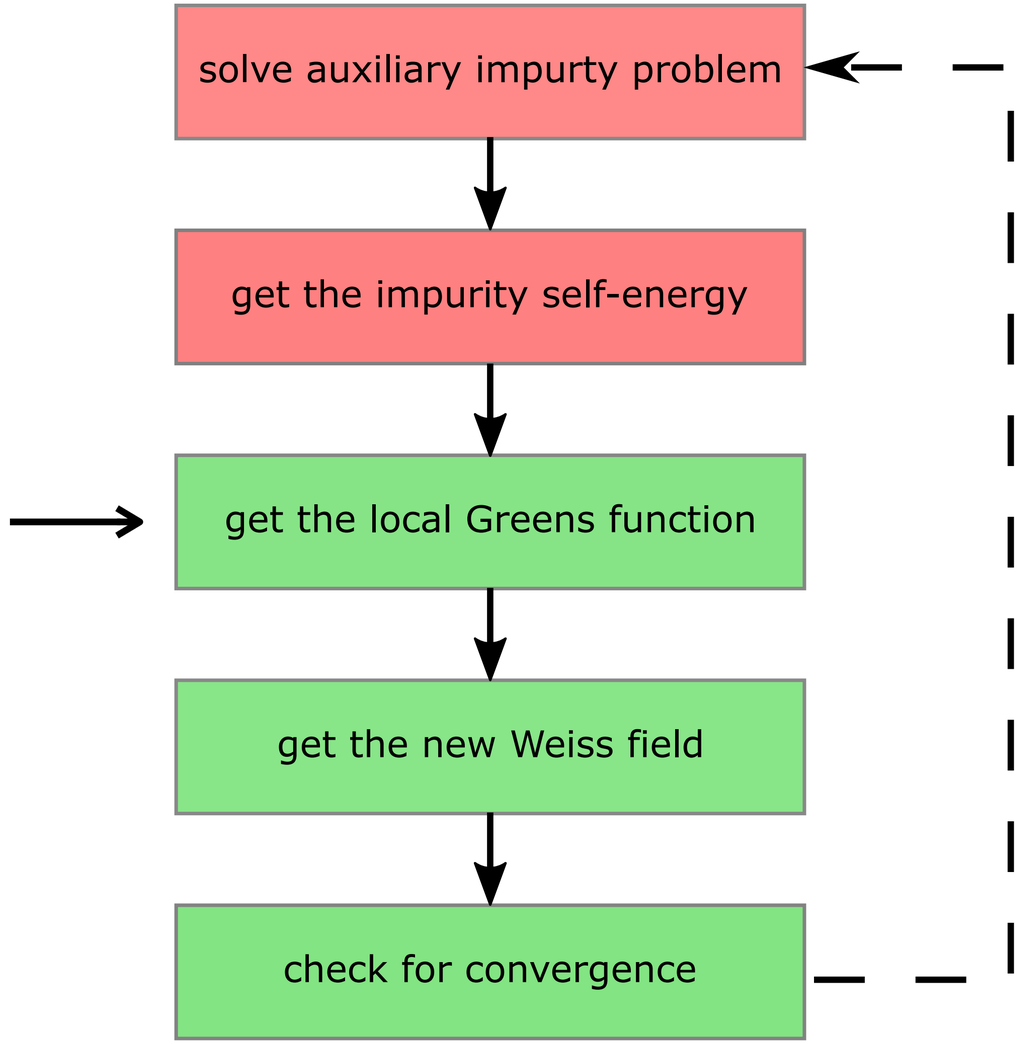
   converged=check_convergence(fg0)
enddo
```

Local greens function

$$G(i\omega_n) = \int d\epsilon \frac{\rho_{\rm bethe}(\epsilon)}{i\omega_n - \epsilon - \Sigma(i\omega)}$$



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   !SELF-CONSISTENCY:
   do i=1,L
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   enddo
   !
   fg0_prev= fg0                          !
   fg0     = one/(one/fg + sigma)
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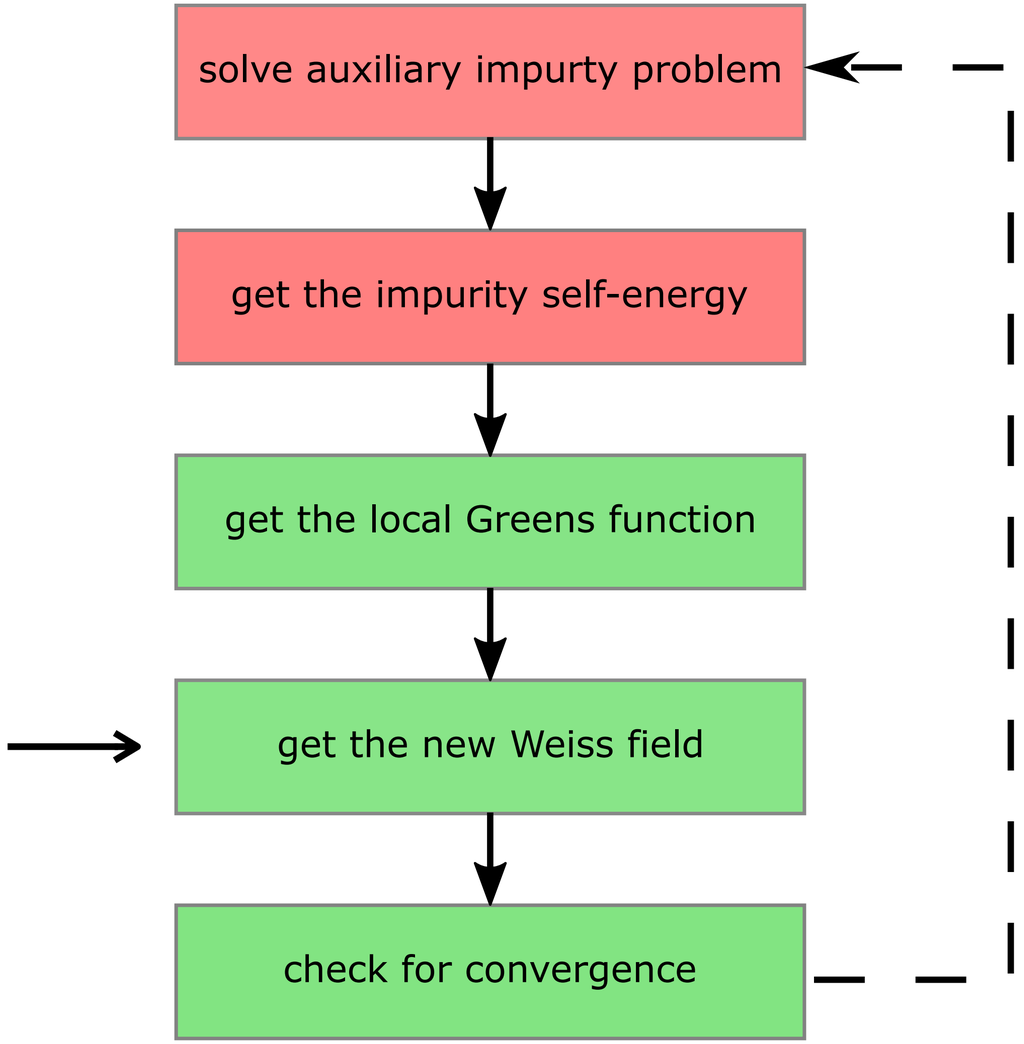
   docc = ipt_measure_docc_matsubara(sigma,fg0)
   write(*,"(3F15.9,3x)",advance="no")dens,docc,z
   !Check CONVERGENCE on the Weiss Field:
   converged=check_convergence(fg0)
enddo
```

$$\mathcal{G}_0^{\text{new}}(i\omega_n) = \frac{1}{G^{-1}(i\omega_n) + \Sigma(i\omega_n)}$$

new Weiss field



ipt_hm_matsubara.f90

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      fg(i) = gfbethe(wm(i),zeta,D)
   enddo
   !
   fg0_prev= fg0                          !
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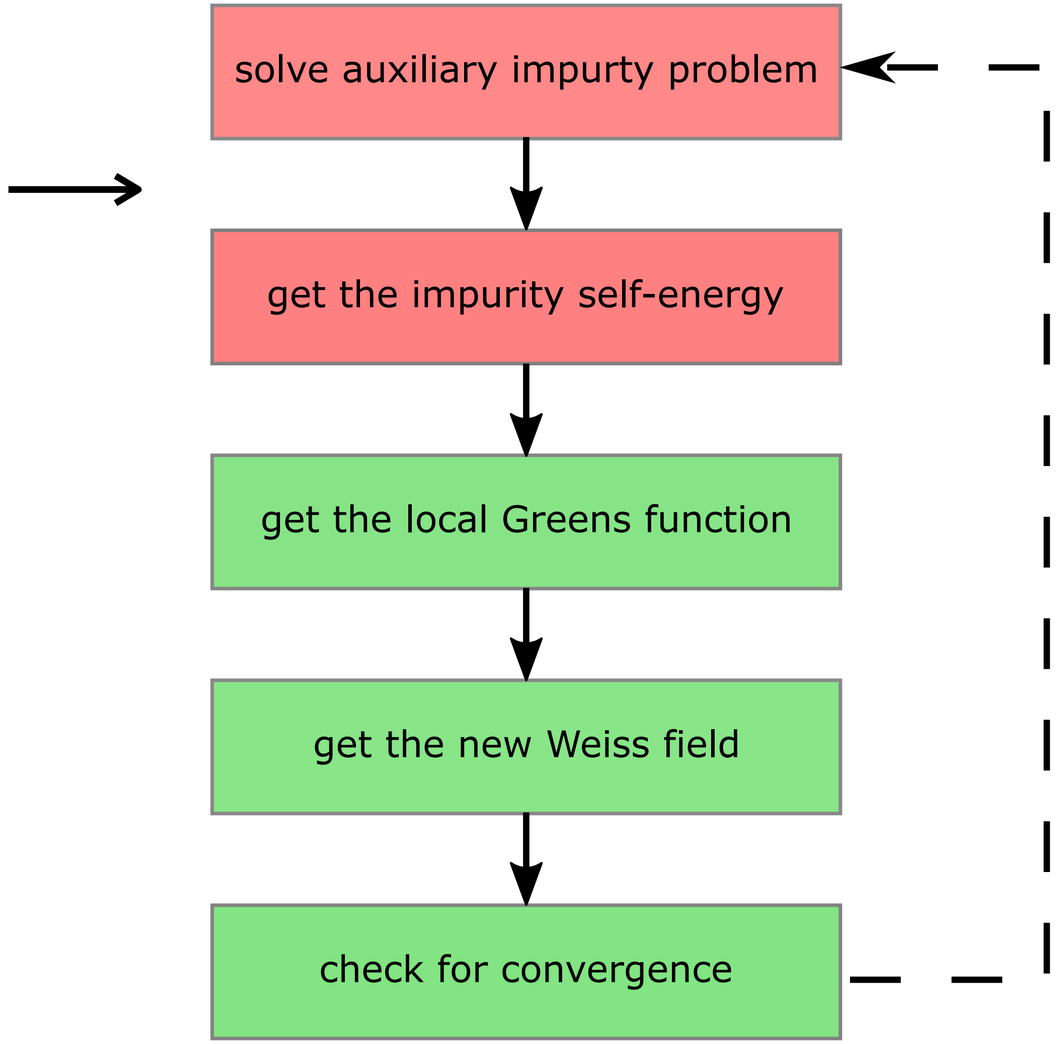
   z    = ipt_measure_zeta_matsubara(sigma,fg0)
   docc = ipt_measure_docc_matsubara(sigma,fg0)
   write(*,"(3F15.9,3x)",advance="no")dens,docc,z
   !Check CONVERGENCE on the Weiss Field:
   converged=check_convergence(fg0)
enddo
```

get the new self-energy



ipt_hm_matsubara.f90

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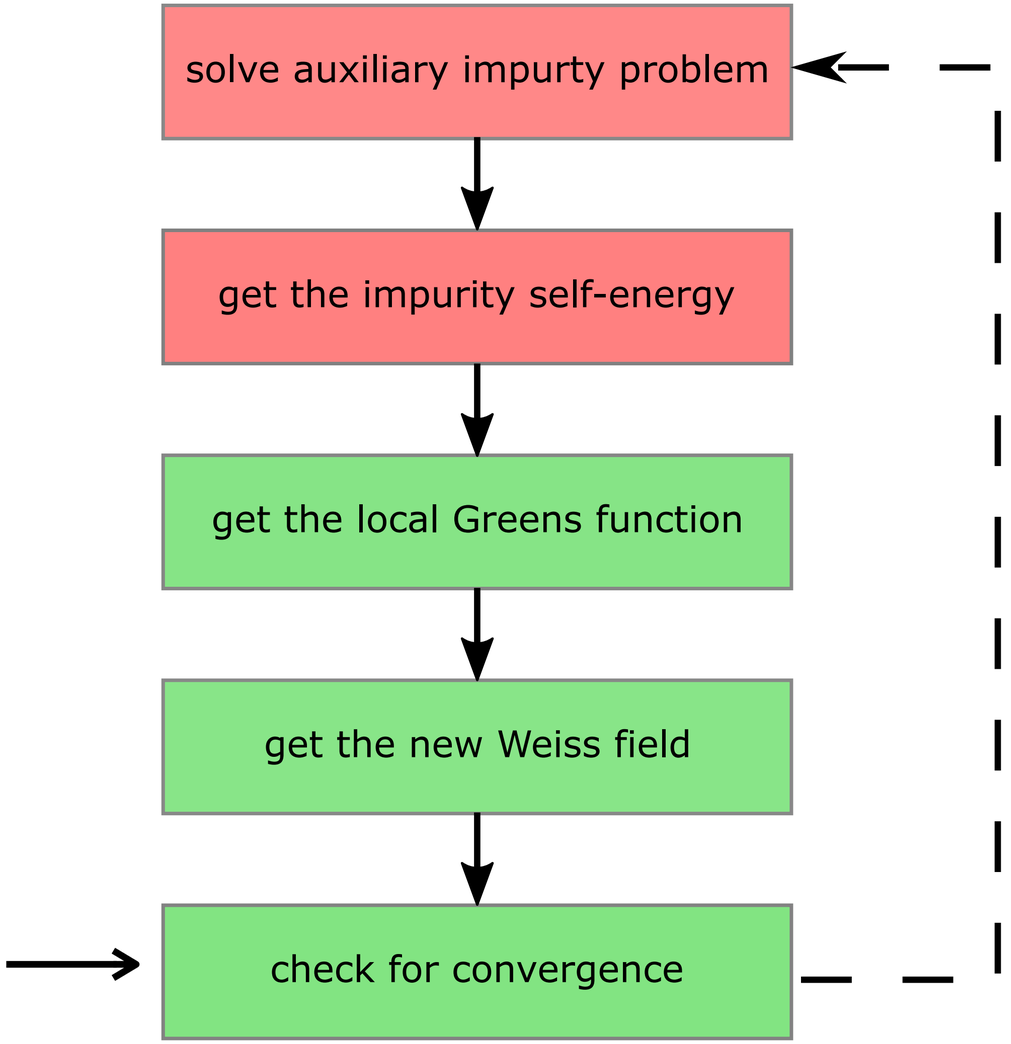
   !SELF-CONSISTENCY:
   do i=1,L
      zeta  = xi*wm(i) - sigma(i)
      fg(i) = gfbethe(wm(i),zeta,D)
   enddo
   !
   fg0_prev= fg0                          !
   fg0     = one/(one/fg + sigma)
   if(iloop>1)fg0 = wmix*fg0 + (1.d0-wmix)*fg0_prev !mix to avoid loops
   !
   !IMPURITY SOLVER: fg0-->sigma
   call solve_ipt_mats(sigma)
   !
   dens = ipt_measure_dens_matsubara(fg)
   z    = ipt_measure_zeta_matsubara(sigma,fg0)
   docc = ipt_measure_docc_matsubara(sigma,fg0)
   write(*,"(3F15.9,3x)",advance="no")dens,docc,z
   !Check CONVERGENCE on the Weiss Field:
   converged=check_convergence(fg0)
enddo
```

measure observable
heck convergence

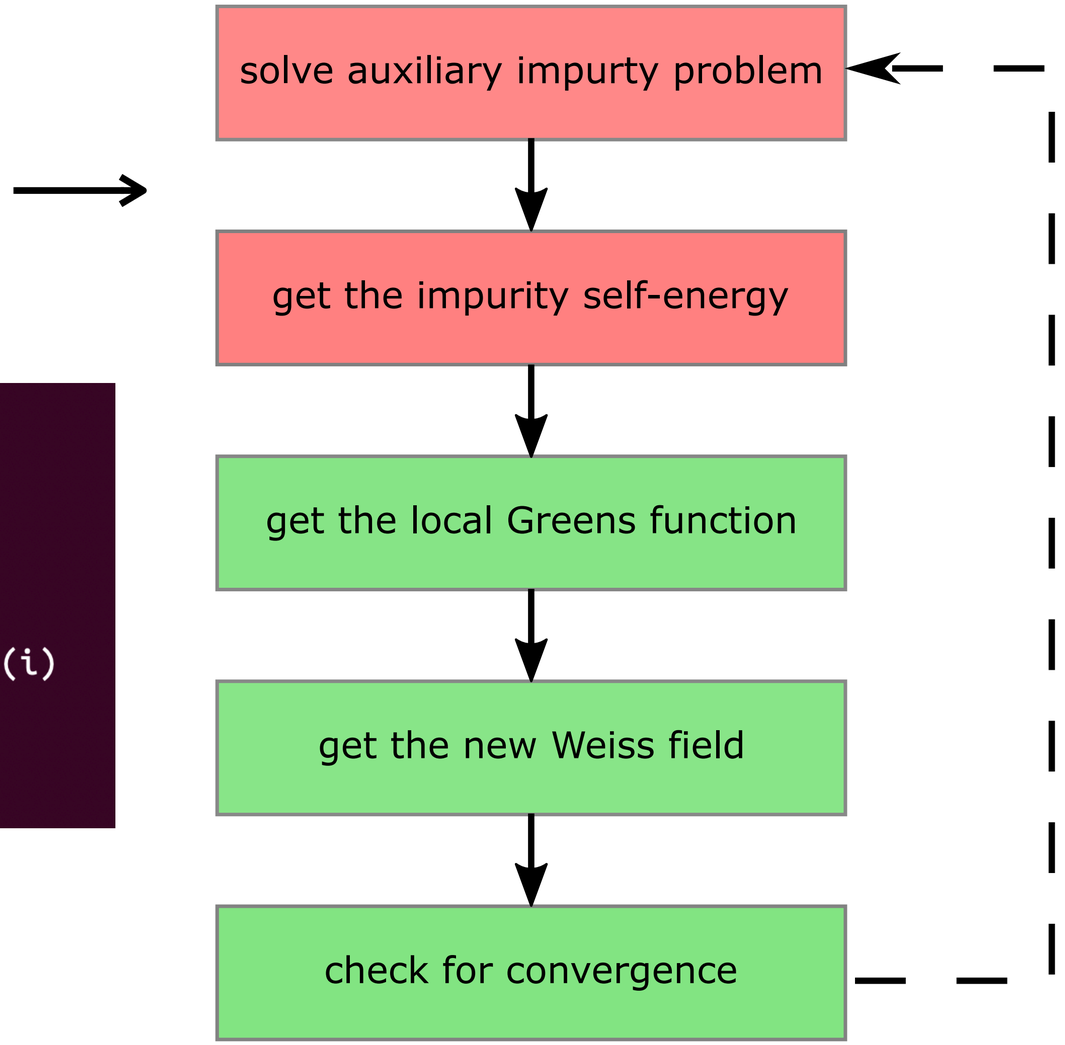


ipt_hm_matsubara.f90

The solver part

```
   !
   !IMPURITY SOLVER: fg0-->sigma
   call solve_ipt_mats(sigma)
   !
```

```
!PURPOSE  : Solve 2^nd order perturbation theory
subroutine solve_ipt_mats(sigma)
  complex(8),dimension(L) :: sigma
  real(8),dimension(0:L)  :: fg0_tau
  real(8),dimension(0:L)  :: sigma_tau
  call fftgf_iw2tau(fg0,fg0_tau(0:),beta)
  forall(i=0:L)sigma_tau(i)=Uloc*Uloc*fg0_tau(i)*fg0_tau(L-i)*fg0_tau(i)
  call fftgf_tau2iw(sigma_tau(0:),Sigma,beta)
  Sigma=xi*dimag(Sigma)
end subroutine solve_ipt_mats
```



ipt_hm_matsubara.f90

inputIPT.conf

```
&IPT_VARIABLE                                    !
NLOOP=300,   max number of DMFTloops              !
ULOC=2.0000000000000000     ,                     !
BETA=100.00000000000000     ,                     !
L=8192 ,
DMFT_ERROR=1.0000000000000000E-005,              !
WMIX=0.5d0,
/                                                !
```

ipt_hm_matsubara.f90

inputIPT.conf

```
&IPT_VARIABLE                                    !
NLOOP=300,                                        !
ULOC=2.0000000000000000      ,   Hubbard U        !
BETA=100.00000000000000      ,                    !
L=8192 ,
DMFT_ERROR=1.0000000000000000E-005,              !
WMIX=0.5d0,
/                                                !
```

ipt_hm_matsubara.f90

inputIPT.conf

```
&IPT_VARIABLE                                    !
NLOOP=300,                                        !
ULOC=2.0000000000000000      ,                    !
BETA=100.00000000000000      , Inverse temperature !
L=8192 ,
DMFT_ERROR=1.0000000000000000E-005,              !
WMIX=0.5d0,
/                                                !
```

ipt_hm_matsubara.f90

inputIPT.conf

```
&IPT_VARIABLE                                    !
NLOOP=300,                                        !
ULOC=2.0000000000000000     ,                     !
BETA=100.00000000000000     ,                     !
L=8192 ,                        number matsubara freq
DMFT_ERROR=1.0000000000000000E-005,               !
WMIX=0.5d0,
/                                                 !
```

ipt_hm_matsubara.f90

inputIPT.conf

```
&IPT_VARIABLE                                    !
NLOOP=300,                                        !
ULOC=2.0000000000000000     ,                     !
BETA=100.00000000000000     ,                     !
L=8192 ,
DMFT_ERROR=1.000000000000000E-005,               !  Threshold for convergence
WMIX=0.5d0,
/                                                !
```

ipt_hm_matsubara.f90

inputIPT.conf

```
&IPT_VARIABLE                                    !
NLOOP=300,                                        !
ULOC=2.0000000000000000     ,                     !
BETA=100.00000000000000     ,                     !
L=8192 ,
DMFT_ERROR=1.0000000000000000E-005,              !
WMIX=0.5d0,                    Mixing parameter
/                                                 !
```

ipt_hm_matsubara.f90

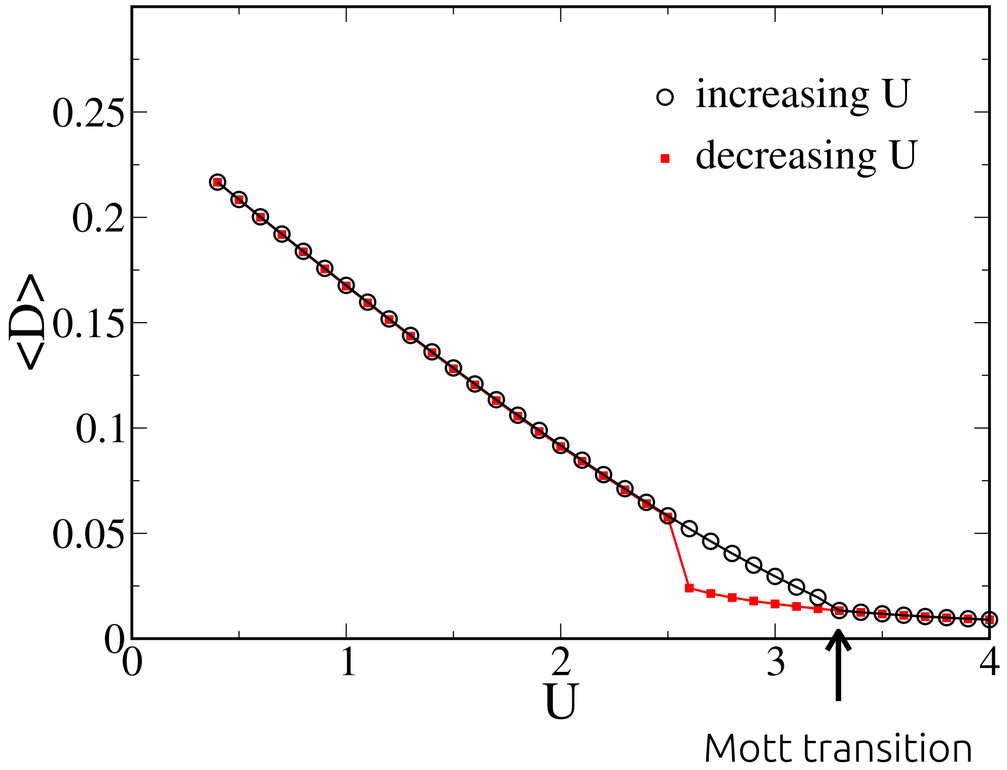
Output

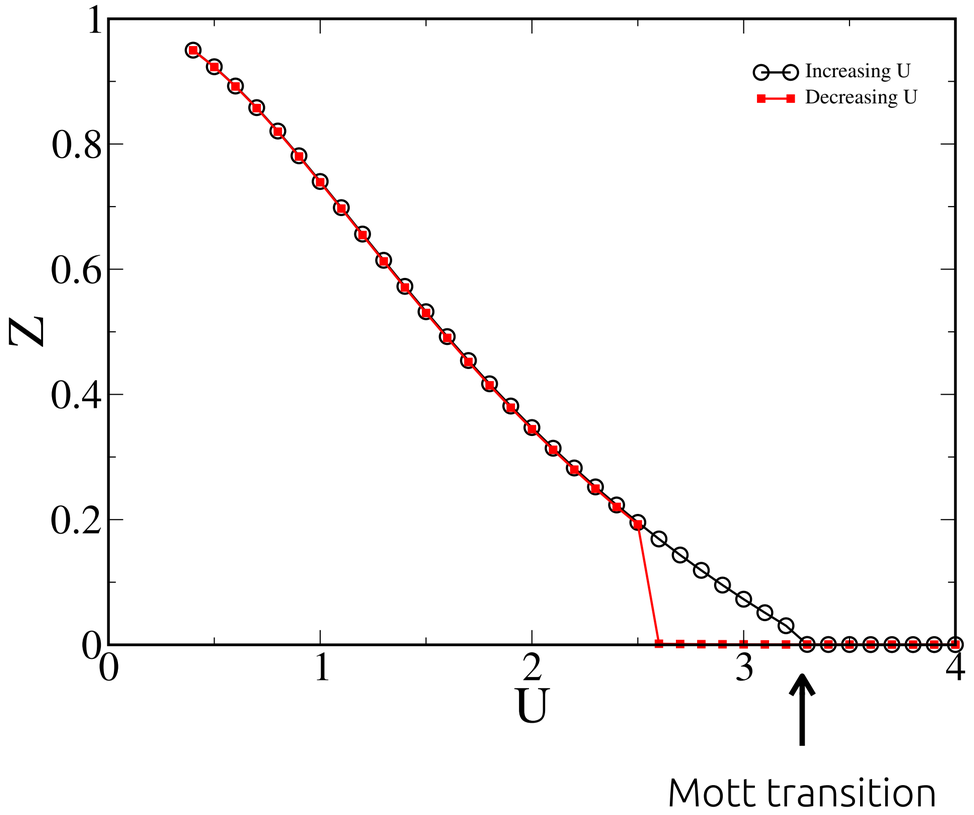
```
&IPT_VARIABLE
 NLOOP=300         ,
 ULOC=  2.0000000000000000     ,
 BETA=  100.00000000000000     ,
 L=8192         ,
 DMFT_ERROR=  1.0000000000000001E-005,
 WMIX= 0.50000000000000000     ,
 /                    ⟨n_iσ⟩          ⟨n_i↑n_i↓⟩      Z = (1 − ∂Σ'/∂ω |ω=0)^−1
DMFT-loop    1    0.500000000    0.111249673    0.433552979   error=  7.3308646E-02
DMFT-loop    2    0.500000000    0.103827550    0.400879447   error=  9.3510057E-03
DMFT-loop    3    0.500000000    0.099227494    0.380916970   error=  5.7538610E-03
DMFT-loop    4    0.500000000    0.096365233    0.368402243   error=  3.6022560E-03
DMFT-loop    5    0.500000000    0.094572993    0.360421234   error=  2.2814657E-03
DMFT-loop    6    0.500000000    0.093443732    0.355276608   error=  1.4563598E-03
DMFT-loop    7    0.500000000    0.092728302    0.351938947   error=  9.3469056E-04
DMFT-loop    8    0.500000000    0.092272972    0.349765678   error=  6.0212279E-04
DMFT-loop    9    0.500000000    0.091982091    0.348347913   error=  3.8888586E-04
DMFT-loop   10    0.500000000    0.091795699    0.347422266   error=  2.5161438E-04
DMFT-loop   11    0.500000000    0.091675965    0.346817817   error=  1.6299983E-04
DMFT-loop   12    0.500000000    0.091598896    0.346423189   error=  1.0568477E-04
DMFT-loop   13    0.500000000    0.091549208    0.346165647   error=  6.8564084E-05
DMFT-loop   14    0.500000000    0.091517130    0.345997648   error=  4.4500045E-05
DMFT-loop   15    0.500000000    0.091496399    0.345888114   error=  2.8890053E-05
DMFT-loop   16    0.500000000    0.091482989    0.345816731   error=  1.8759520E-05
DMFT-loop   17    0.500000000    0.091474309    0.345770233   error=  1.2182984E-05
DMFT-loop   18    0.500000000    0.091468686    0.345739956   error=  7.9127131E-06
DMFT-loop   19    0.500000000    0.091465042    0.345720248   error=  5.1395346E-06
```

Output files

```
[giacomo@hyperion 12:
G0_iw.ipt
G_iw.ipt
Sigma.restart
Sigma_iw.ipt
inputIPT.conf
observables_last.ipt
```

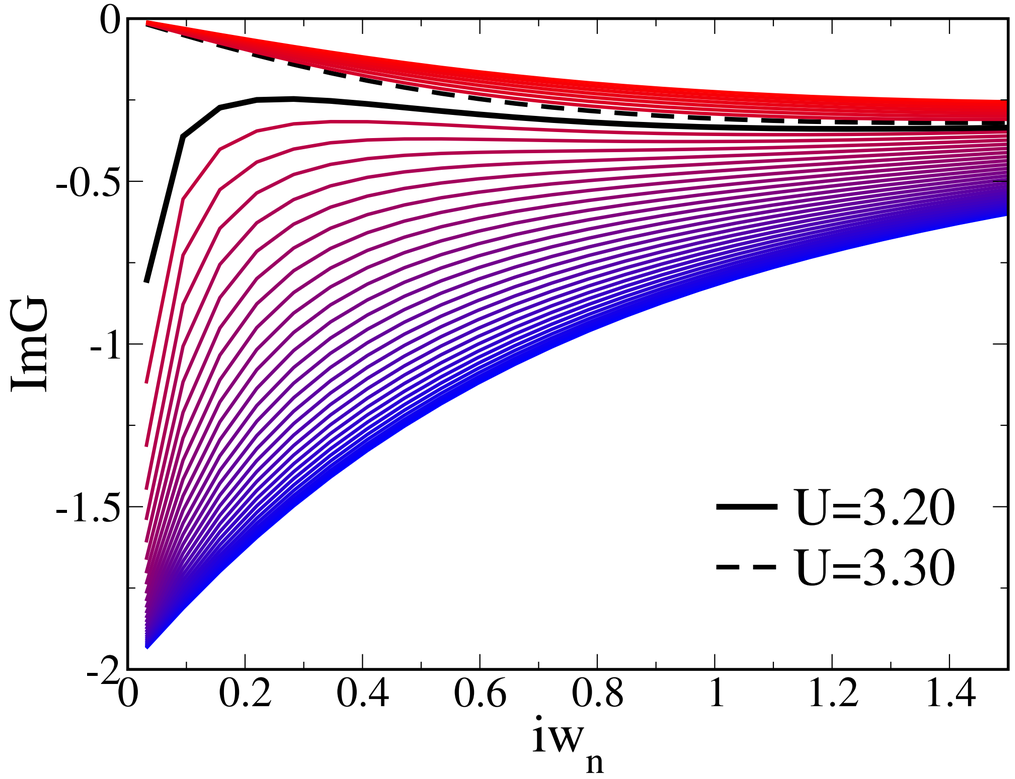
Example: run the code at different U adiabatically following the solution

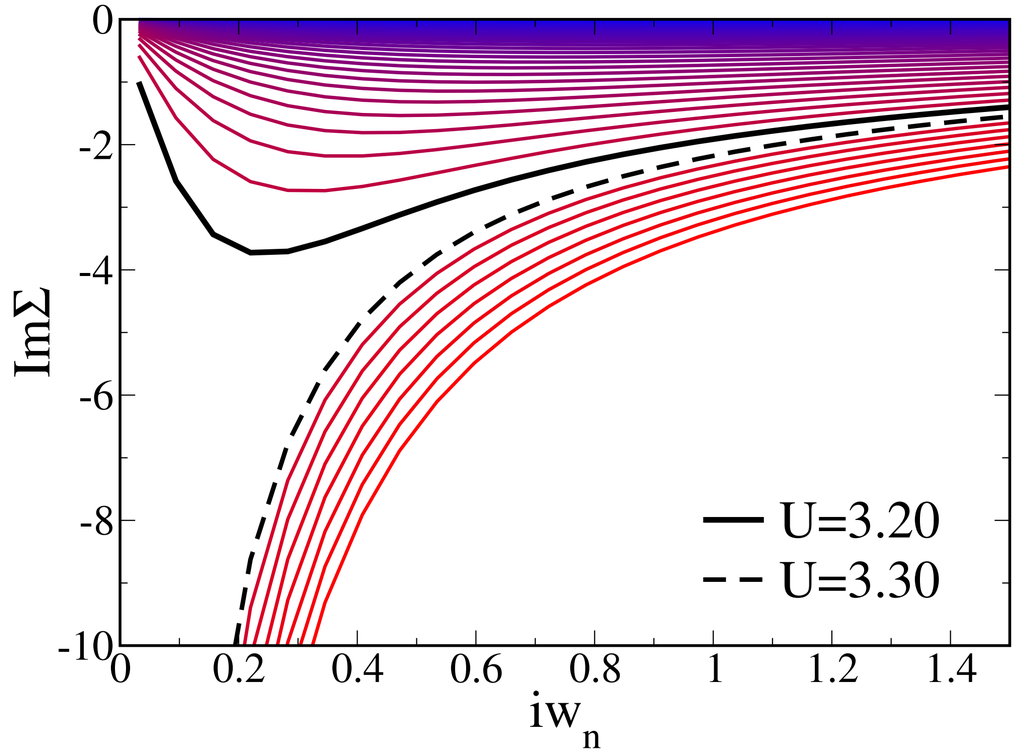




For fun: change the temperature and check that the Mott transition becomes first order

Green’s function and self-energies VS imaginary frequencies





For fun: change the temperature and check that the Mott transition becomes first order

ipt_hm_real.f90

```
!dmft loop:
iloop=0 ; converged=.false.
do while(.not.converged.AND.iloop<nloop)
   iloop=iloop+1
   write(*,"(A,i5,A)",advance="no")"DMFT-loop",iloop," "
   !
   !
   !SELF-CONSISTENCY:
   do i=1,L
      zeta = dcmplx(wr(i),eps) - sigma(i)
      fg(i) = gfbether(wr(i),zeta,D)
   enddo
   !
   fg0_prev= fg0                                    !
   fg0     = one/(one/fg + sigma)                   !
   if(iloop>1)fg0 = wmix*fg0 + (1.d0-wmix)*fg0_prev !mix to avoid loops
   !
   !IMPURITY SOLVER: fg0-->sigma
   call solve_ipt_real(sigma)
   !
   !Check CONVERGENCE on the Weiss Field:
   converged=check_convergence(fg0)
enddo
```

$i\omega_n \rightarrow \omega + i0^+$

real freq solver

```
&IPT_VARIABLE                                      !
NLOOP=300,                                          !
ULOC=2.0000000      ,                   !
BETA=100.00000000000000     ,                      !
L=2000,
DMFT_ERROR=1.0000000000000001E-004,                 !
WMIX=0.5d0,
EPS=0.01d0,
/                                                   !
```

real frequency discretisation

Imaginary broadening

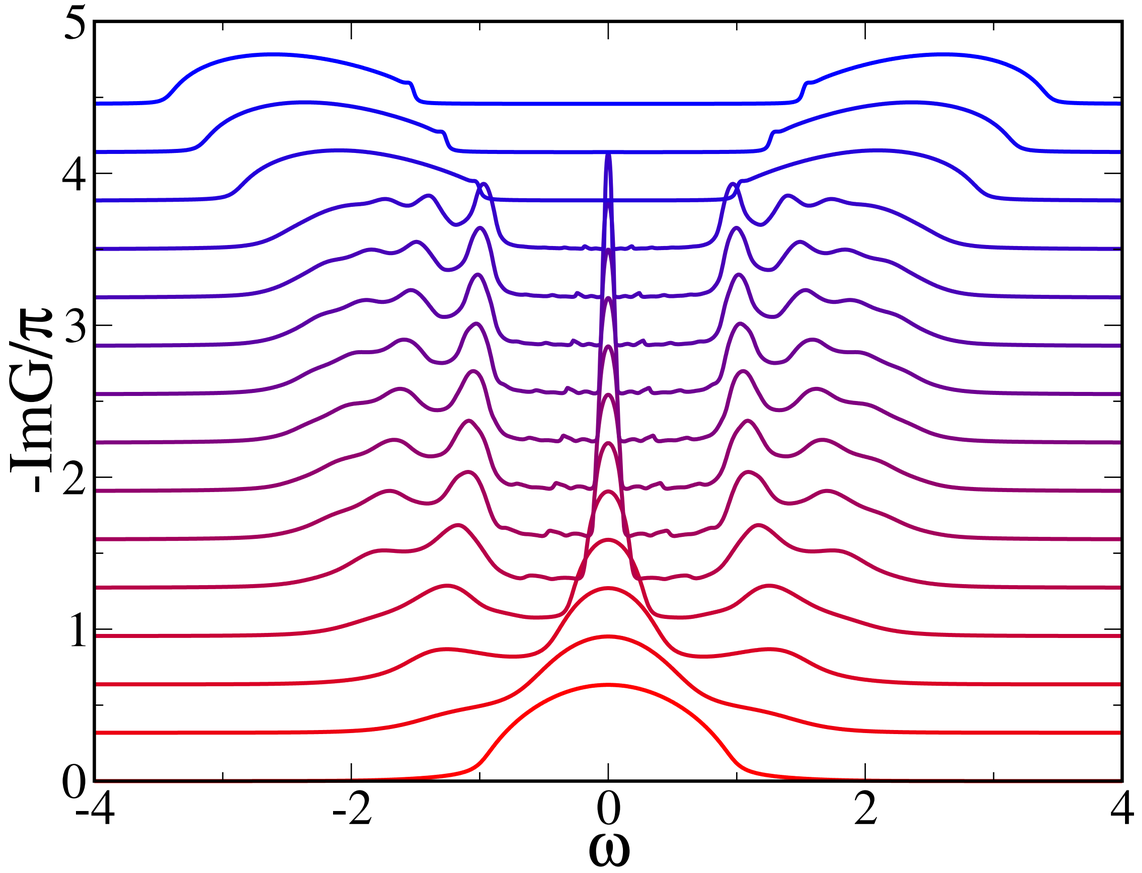
```
!PURPOSE  : Solve 2^nd order perturbation theory
subroutine solve_ipt_real(sigma)
  complex(8),dimension(L) :: sigma
  integer                 :: ix,iy,iz
  real(8)                 :: sum1,sum2
  real(8),dimension(L)    :: reS,imS
  !
  call getAs
  call getPolarization
  !
  do ix=1,L
     sum1=zero
     sum2=zero
     do iy=1,L
        iz= iy_m_ix(iy,ix)
        if(iz>0)then
           sum1=sum1+A0p(iy)*P1(iz)*mesh
           sum2=sum2+A0m(iy)*P2(iz)*mesh
        end if
     enddo
     imS(ix)=-Uloc*Uloc*(sum1+sum2)*pi
  enddo
  reS   = kronig(imS,wr,L)
  sigma = reS + xi*imS
end subroutine solve_ipt_real
```

real freq solver

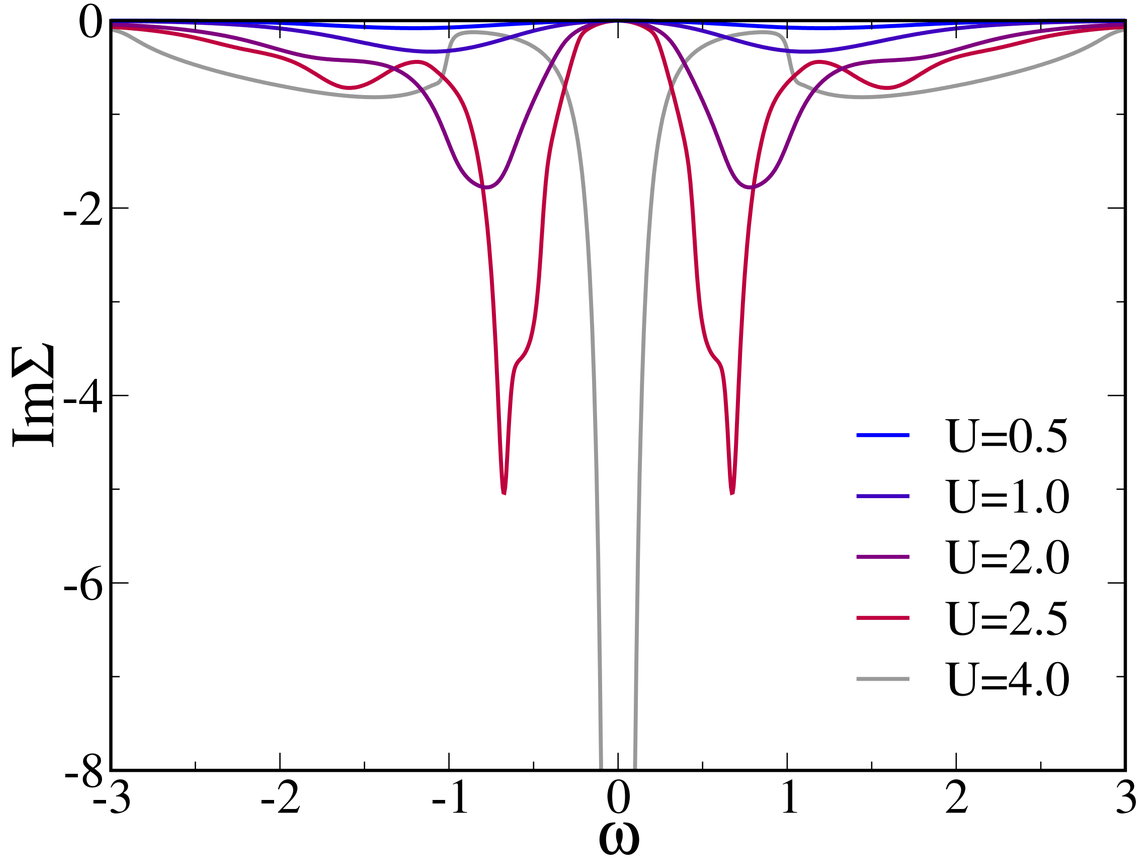
Frequency convolutions
In the sunset diagram

The real frequency solver gives access at the spectral functions

Formation of the Mott gap



Fermi liquid VS non-fermi liquid self-energies

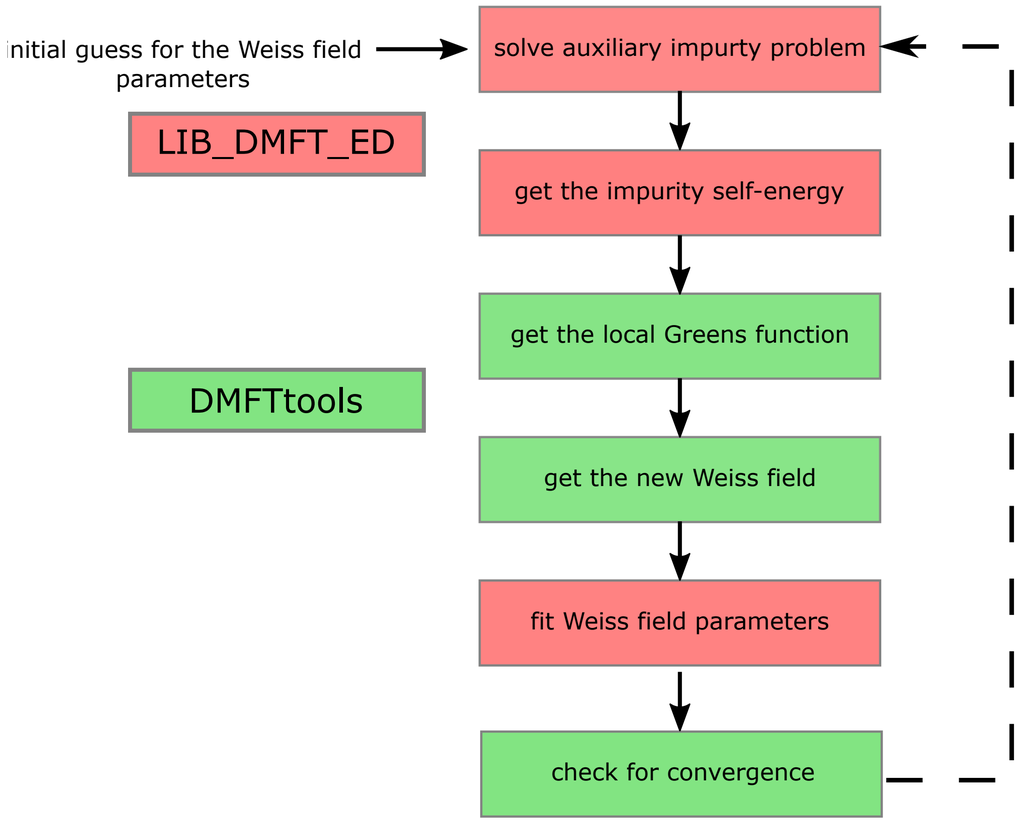


Exact Diagonalization solver

$$H_{imp} = U n_{i\uparrow} n_{i\downarrow} - \mu \sum_{\sigma} n_{i\sigma} + \sum_{l\sigma} v_l c^{\dagger}_{i\sigma} d_{l\sigma} + h.c. + \sum_{l} \varepsilon_l d^{\dagger}_{l\sigma} d_{l\sigma}$$

$$\Delta(i\omega_n) = \sum_{l} \frac{|v_l|^2}{i\omega_n - \varepsilon_l}$$

$$\mathcal{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \Delta(i\omega_n)$$

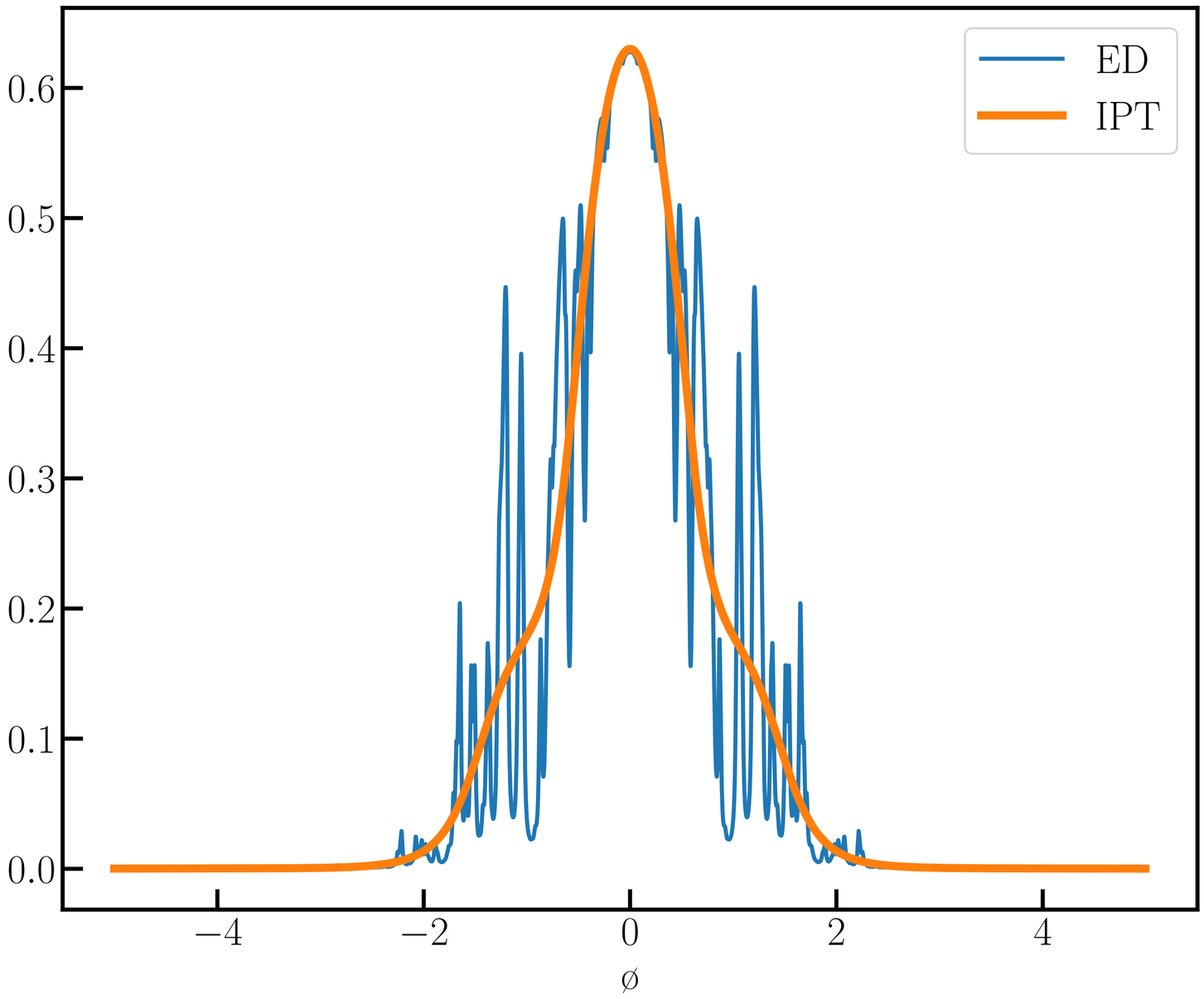


1. Find the ground state of H_imp → Lanczos method
2. Compute the Green's function

Minimize a cost function to get the new bath parameters

$$\chi^2[\{\varepsilon_l, v_l\}] = \sum_{\omega_n} w_n |\Delta(i\omega_n; \{\varepsilon_l, v_l\}) - \Delta_{\text{target}}(i\omega_n)|^2$$

!!!! ED is not good for real axis calculations !!!!


ED
IPT
0.6
0.5
0.4
0.3
0.2
0.1
0.0
−4
−2
0
2
4
ø

DMFT equations for superconductivity

Replace all the Green's function by matrix Green's functions in the Nambu representation

$$\mathbf{G}_{ii} = \begin{pmatrix} -\langle T_\tau c_{i\uparrow}(\tau) c^\dagger_{i\uparrow}(\tau')\rangle & -\langle T_\tau c^\dagger_{i\uparrow}(\tau) c^\dagger_{i\downarrow}(\tau')\rangle \\ -\langle T_\tau c_{i\downarrow}(\tau) c_{i\uparrow}(\tau')\rangle & -\langle T_\tau c^\dagger_{i\downarrow}(\tau) c_{i\downarrow}(\tau')\rangle \end{pmatrix} = \begin{pmatrix} G_{\uparrow\uparrow}(\tau-\tau') & F_{\uparrow\downarrow}(\tau-\tau') \\ \overline{F}_{\downarrow\uparrow}(\tau-\tau') & \overline{G}_{\downarrow\downarrow}(\tau-\tau') \end{pmatrix}$$

$G_{\uparrow\uparrow}(\tau-\tau')$ $\quad$ $\overline{G}_{\downarrow\downarrow}(\tau-\tau')$ $\quad$ Normal Green's function

$F_{\uparrow\downarrow}(\tau-\tau')$ $\quad$ $\overline{F}_{\downarrow\uparrow}(\tau-\tau')$ $\quad$ Anomalous Green's function

Same for Weiss field and Self-energy

$$H^{SC}_{imp} = U n_{i\uparrow} n_{i\downarrow} - \mu \sum_\sigma n_{i\sigma} + \sum_{l\sigma} v_l c^\dagger_{i\sigma} d_{l\sigma} + h.c. + \sum_l \varepsilon_l d^\dagger_{l\sigma} d_{l\sigma} + \sum_l \Delta_l d^\dagger_{l\uparrow} d^\dagger_{l\downarrow} + h.c$$

extra parameter in the impurity Hamiltonian
Allow for SC symmetry breaking in the Weiss field

ed_ahm_bethe.f90 driver (*) to solve the (attractive) Hubbard model on the bethe lattice

$$H = -t \sum_{ij} c^{\dagger}_{i\sigma} c_{i\sigma} - |U| \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma}$$

Prototype model for unconventional (ie non BCS) superconductivity (s-wave)

(*) driver = small program that makes use of the routines in the Libraries DMFTtools and LIB_DMFT_ET

Different physical problems may need slightly different sets of instructions

If you want to study a different problem then you may need to write a specific driver

The driver ed_ahm_bethe.f90 is quite general and it represents a good starting point for any physical problem

****If you want to use this code in your research please cite ***

Amaricci et al, "EDIpack: A parallel exact diagonalization package for quantum impurity problems" arXiv 2105.06806

ed_ahm_bethe.f90 solve the attractive Hubbard model on the be the Lattice

```
!
!Allocate local functions (Nambu)
allocate(Gmats(2,Nspin,Nspin,Norb,Norb,Lmats))
allocate(Smats(2,Nspin,Nspin,Norb,Norb,Lmats))
allocate(Weiss(2,Nspin,Nspin,Norb,Norb,Lmats))
!
allocate(Greal(2,Nspin,Nspin,Norb,Norb,Lreal))
allocate(Sreal(2,Nspin,Nspin,Norb,Norb,Lreal))
!
allocate(Ebethe(1,Le))
Ebethe(1,:) = linspace(-Wband,Wband,Le,mesh=de)
!
allocate(Dbethe(1,Le))
Dbethe(1,:) = dens_bethe(Ebethe(1,:),wband)*de
!
allocate(Hloc(1,1,1,1))
Hloc        = 0d0
!
allocate(H0(1))
H0=0d0
!
!Setup solver
Nb=ed_get_bath_dimension()
allocate(Bath(Nb))
allocate(Bath_prev(Nb))
call ed_init_solver(bath)
```

Allocate normal AND anomalous
Greens Functions/Weiss field/Self energy

ed_ahm_bethe.f90 solve the attractive Hubbard model on the be the Lattice

```
!
!Allocate local functions (Nambu)
allocate(Gmats(2,Nspin,Nspin,Norb,Norb,Lmats))
allocate(Smats(2,Nspin,Nspin,Norb,Norb,Lmats))
allocate(Weiss(2,Nspin,Nspin,Norb,Norb,Lmats))
!
allocate(Greal(2,Nspin,Nspin,Norb,Norb,Lreal))
allocate(Sreal(2,Nspin,Nspin,Norb,Norb,Lreal))
!
allocate(Ebethe(1,Le))
Ebethe(1,:) = linspace(-Wband,Wband,Le,mesh=de)
!
allocate(Dbethe(1,Le))
Dbethe(1,:) = dens_bethe(Ebethe(1,:),wband)*de
!
allocate(Hloc(1,1,1,1))
Hloc        = 0d0
!
allocate(H0(1))
H0=0d0
!
!Setup solver
Nb=ed_get_bath_dimension()
allocate(Bath(Nb))
allocate(Bath_prev(Nb))
call ed_init_solver(bath)
```

Set the density of states of the Bethe lattice

Set the energy of the atomic levels (here 0)

ed_ahm_bethe.f90 solve the attractive Hubbard model on the be the Lattice

```
!
!Allocate local functions (Nambu)
allocate(Gmats(2,Nspin,Nspin,Norb,Norb,Lmats))
allocate(Smats(2,Nspin,Nspin,Norb,Norb,Lmats))
allocate(Weiss(2,Nspin,Nspin,Norb,Norb,Lmats))
!
allocate(Greal(2,Nspin,Nspin,Norb,Norb,Lreal))
allocate(Sreal(2,Nspin,Nspin,Norb,Norb,Lreal))
!
allocate(Ebethe(1,Le))
Ebethe(1,:) = linspace(-Wband,Wband,Le,mesh=de)
!
allocate(Dbethe(1,Le))
Dbethe(1,:) = dens_bethe(Ebethe(1,:),wband)*de
!
allocate(Hloc(1,1,1,1))
Hloc        = 0d0
!
allocate(H0(1))
H0=0d0
!
!Setup solver
Nb=ed_get_bath_dimension()
allocate(Bath(Nb))
allocate(Bath_prev(Nb))
call ed_init_solver(bath)
```

"baths" = $\{\varepsilon_l, v_l, \Delta_l\}$

Allocate the bath at loop iloop
Allocate the bath at loop iloop+1

Set-up and init the solver

ed_ahm_bethe.f90 solve the attractive Hubbard model on the be the Lattice

```
!DMFT loop
iloop=0;converged=.false.
do while(.not.converged.AND.iloop<nloop)
   iloop=iloop+1
   call start_loop(iloop,nloop,"DMFT-loop")
   !Solve the EFFECTIVE IMPURITY PROBLEM (first w/ a guess for the bath)
   call ed_solve(bath,Hloc)
   !Retrieve impurity self-energies (normal, anomalous)
   call ed_get_Sigma_matsubara(Smats(1,:,:,:,:,:))
   call ed_get_Self_matsubara(Smats(2,:,:,:,:,:))
   call ed_get_Sigma_realaxis(Sreal(1,:,:,:,:,:))
   call ed_get_Self_realaxis(Sreal(2,:,:,:,:,:))
   call ed_get_dens(dens,iorb=1)

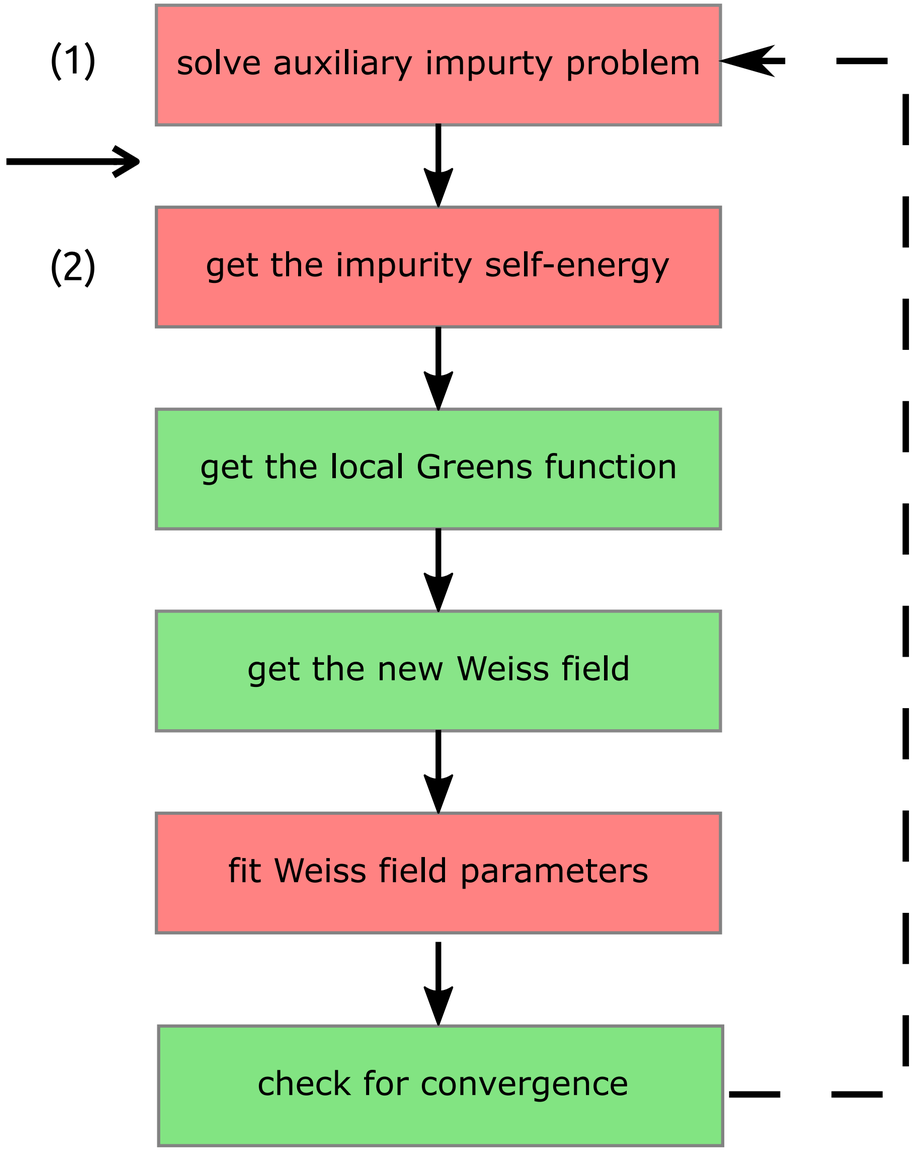
   !Compute the local gfs:
   call dmft_gloc_matsubara(Ebethe,Dbethe,H0,Gmats,Smats)

   call dmft_self_consistency(Gmats(1,:,:,:,:,:),Gmats(2,:,:,:,:,:),&
        Smats(1,:,:,:,:,:),Smats(2,:,:,:,:,:),&
        Weiss(1,:,:,:,:,:),Weiss(2,:,:,:,:,:),&
        Hloc,trim(cg_scheme))
   call dmft_print_gf_matsubara(Gmats(1,:,:,:,:,:),"Gloc",iprint=1)
   call dmft_print_gf_matsubara(Gmats(2,:,:,:,:,:),"Floc",iprint=1)
   call dmft_print_gf_matsubara(Weiss(1,:,:,:,:,:),"Weiss",iprint=1)
   call dmft_print_gf_matsubara(Weiss(2,:,:,:,:,:),"fWeiss",iprint=1)
   !Perform the self-consistency fitting the new bath
   call ed_chi2_fitgf(Weiss,bath,ispin=1)
   !if it holds apply symmetrizations
   if(phsym)call ed_ph_symmetrize_bath(bath,save=.true.)
   if(normal_bath)call ed_enforce_normal_bath(bath,save=.true.)
   !MIXING:
   if(iloop>1)Bath = wmixing*Bath + (1.d0-wmixing)*Bath_prev
   Bath_prev=Bath
   !Check convergence (if required change chemical potential)
   converged = check_convergence(Weiss(1,1,1,1,1,:),dmft_error,nsuccess,nloop,reset=.false.)
   if(nread/=0.d0)call ed_search_variable(xmu,dens,converged)
   !Close this DMFT loop
   call end_loop
enddo
```

(1) find the ground state of H_imp

(2) compute GF

solver part



ed_ahm_bethe.f90 solve the attractive Hubbard model on the be the Lattice

```
!DMFT loop
iloop=0;converged=.false.
do while(.not.converged.AND.iloop<nloop)
   iloop=iloop+1
   call start_loop(iloop,nloop,"DMFT-loop")
   !Solve the EFFECTIVE IMPURITY PROBLEM (first w/ a guess for the bath)
   call ed_solve(bath,Hloc)

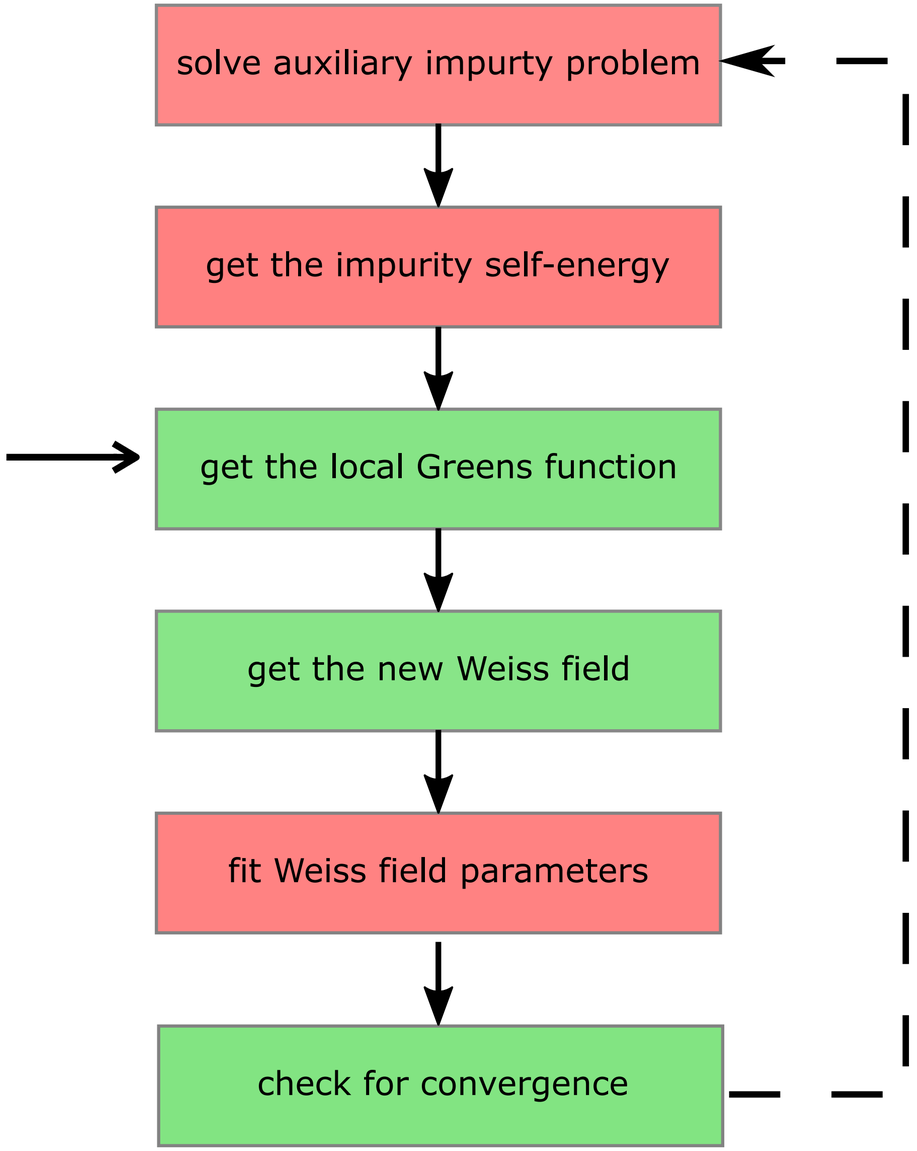
   !Retrieve impurity self-energies (normal, anomalous)
   call ed_get_Sigma_matsubara(Smats(1,:,:,:,:,:))
   call ed_get_Self_matsubara(Smats(2,:,:,:,:,:))
   call ed_get_Sigma_realaxis(Sreal(1,:,:,:,:,:))
   call ed_get_Self_realaxis(Sreal(2,:,:,:,:,:))
   call ed_get_dens(dens,iorb=1)

   !Compute the local gfs:
   call dmft_gloc_matsubara(Ebethe,Dbethe,H0,Gmats,Smats)

   call dmft_self_consistency(Gmats(1,:,:,:,:,:),Gmats(2,:,:,:,:,:),&
        Smats(1,:,:,:,:,:),Smats(2,:,:,:,:,:),&
        Weiss(1,:,:,:,:,:),Weiss(2,:,:,:,:,:),&
        Hloc,trim(cg_scheme))
   call dmft_print_gf_matsubara(Gmats(1,:,:,:,:,:),"Gloc",iprint=1)
   call dmft_print_gf_matsubara(Gmats(2,:,:,:,:,:),"Floc",iprint=1)
   call dmft_print_gf_matsubara(Weiss(1,:,:,:,:,:),"Weiss",iprint=1)
   call dmft_print_gf_matsubara(Weiss(2,:,:,:,:,:),"fWeiss",iprint=1)
   !Perform the self-consistency fitting the new bath
   call ed_chi2_fitgf(Weiss,bath,ispin=1)
   !if it holds apply symmetrizations
   if(phsym)call ed_ph_symmetrize_bath(bath,save=.true.)
   if(normal_bath)call ed_enforce_normal_bath(bath,save=.true.)
   !MIXING:
   if(iloop>1)Bath = wmixing*Bath + (1.d0-wmixing)*Bath_prev
   Bath_prev=Bath
   !Check convergence (if required change chemical potential)
   converged = check_convergence(Weiss(1,1,1,1,1,:),dmft_error,nsuccess,nloop,reset=.false.)
   if(nread/=0.d0)call ed_search_variable(xmu,dens,converged)
   !Close this DMFT loop
   call end_loop
enddo
```

$$G(i\omega_n) = \int d\epsilon \frac{\rho_{\text{bethe}}(\epsilon)}{i\omega_n - \epsilon - \Sigma(i\omega)}$$

Get the local GF



ed_ahm_bethe.f90 solve the attractive Hubbard model on the be the Lattice

```
!DMFT loop
iloop=0;converged=.false.
do while(.not.converged.AND.iloop<nloop)
   iloop=iloop+1
   call start_loop(iloop,nloop,"DMFT-loop")
   !Solve the EFFECTIVE IMPURITY PROBLEM (first w/ a guess for the bath)
   call ed_solve(bath,Hloc)

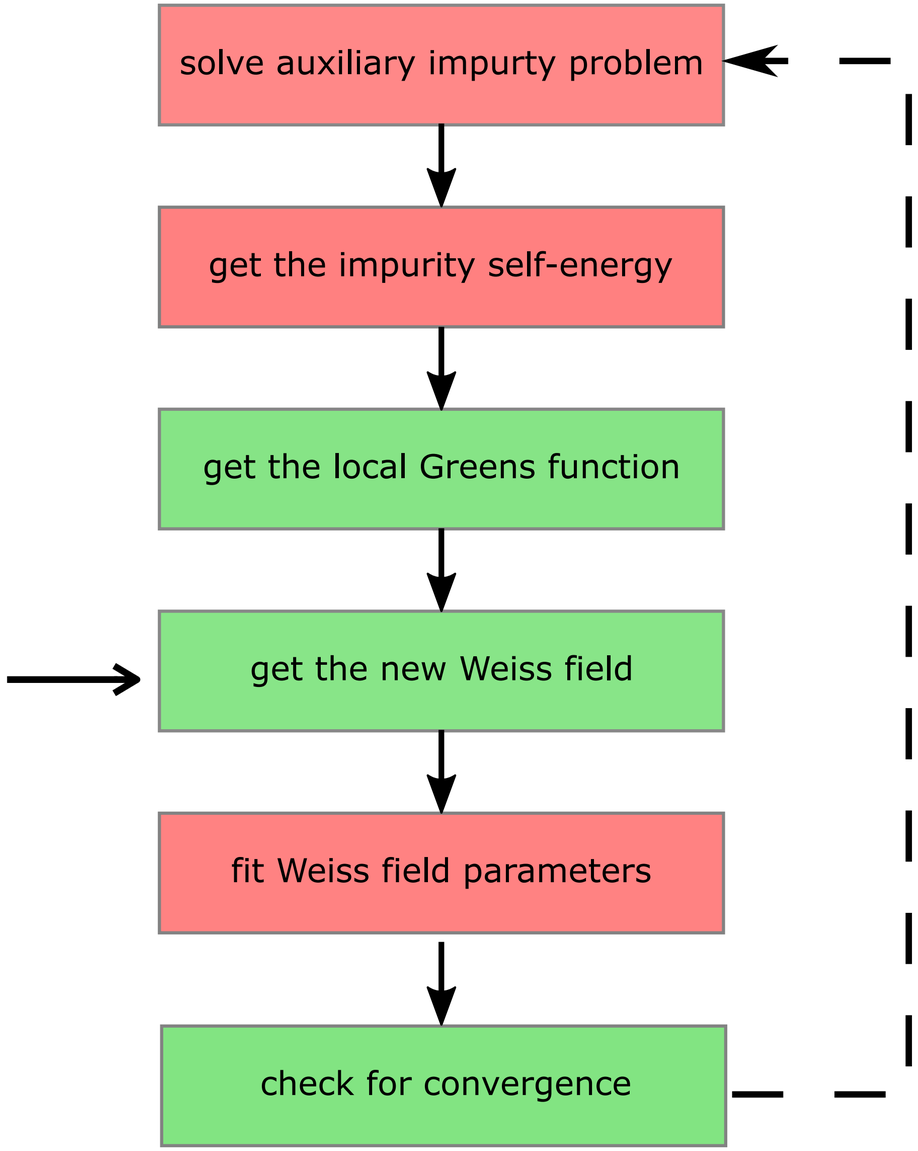
   !Retrieve impurity self-energies (normal, anomalous)
   call ed_get_Sigma_matsubara(Smats(1,:,:,:,:,:,:))
   call ed_get_Self_matsubara(Smats(2,:,:,:,:,:,:))
   call ed_get_Sigma_realaxis(Sreal(1,:,:,:,:,:,:))
   call ed_get_Self_realaxis(Sreal(2,:,:,:,:,:,:))
   call ed_get_dens(dens,iorb=1)

   !Compute the local gfs:
   call dmft_gloc_matsubara(Ebethe,Dbethe,H0,Gmats,Smats)

   call dmft_self_consistency(Gmats(1,:,:,:,:,:,:),Gmats(2,:,:,:,:,:,:),&
        Smats(1,:,:,:,:,:,:),Smats(2,:,:,:,:,:,:),&
        Weiss(1,:,:,:,:,:,:),Weiss(2,:,:,:,:,:,:),&
        Hloc,trim(cg_scheme))
   call dmft_print_gf_matsubara(Gmats(1,:,:,:,:,:,:),"Gloc",iprint=1)
   call dmft_print_gf_matsubara(Gmats(2,:,:,:,:,:,:),"Floc",iprint=1)
   call dmft_print_gf_matsubara(Weiss(1,:,:,:,:,:,:),"Weiss",iprint=1)
   call dmft_print_gf_matsubara(Weiss(2,:,:,:,:,:,:),"fWeiss",iprint=1)
   !Perform the self-consistency fitting the new bath
   call ed_chi2_fitgf(Weiss,bath,ispin=1)
   !if it holds apply symmetrizations
   if(phsym)call ed_ph_symmetrize_bath(bath,save=.true.)
   if(normal_bath)call ed_enforce_normal_bath(bath,save=.true.)
   !MIXING:
   if(iloop>1)Bath = wmixing*Bath + (1.d0-wmixing)*Bath_prev
   Bath_prev=Bath
   !Check convergence (if required change chemical potential)
   converged = check_convergence(Weiss(1,1,1,1,1,:),dmft_error,nsuccess,nloop,reset=.false.)
   if(nread/=0.d0)call ed_search_variable(xmu,dens,converged)
   !Close this DMFT loop
   call end_loop
enddo
```

$$\mathcal{G}_0^{\rm new}(i\omega_n) = \frac{1}{G^{-1}(i\omega_n) + \Sigma(i\omega_n)}$$

Get the new Weiss field



ed_ahm_bethe.f90 solve the attractive Hubbard model on the be the Lattice

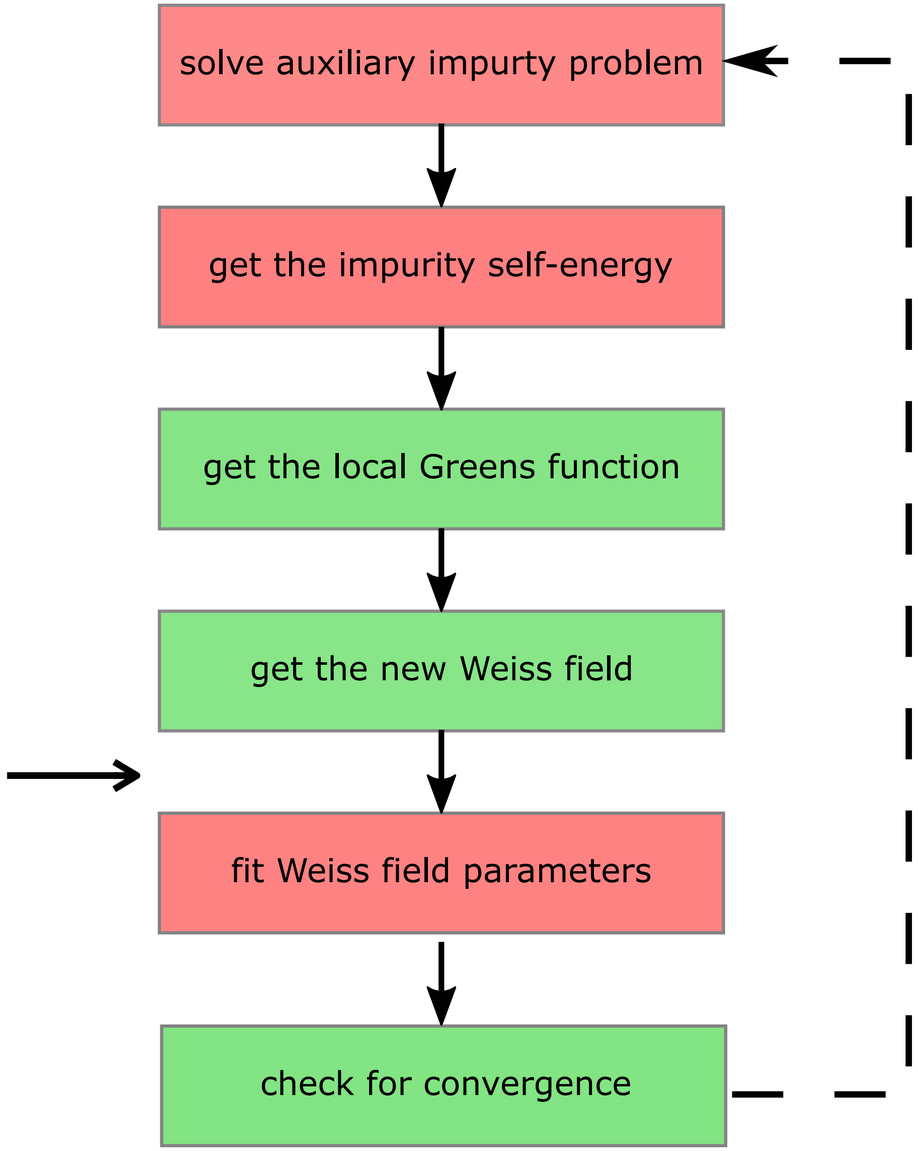
```
!DMFT loop
iloop=0;converged=.false.
do while(.not.converged.AND.iloop<nloop)
   iloop=iloop+1
   call start_loop(iloop,nloop,"DMFT-loop")
   !Solve the EFFECTIVE IMPURITY PROBLEM (first w/ a guess for the bath)
   call ed_solve(bath,Hloc)

   !Retrieve impurity self-energies (normal, anomalous)
   call ed_get_Sigma_matsubara(Smats(1,:,:,:,:,:,:))
   call ed_get_Self_matsubara(Smats(2,:,:,:,:,:,:))
   call ed_get_Sigma_realaxis(Sreal(1,:,:,:,:,:,:))
   call ed_get_Self_realaxis(Sreal(2,:,:,:,:,:,:))
   call ed_get_dens(dens,iorb=1)

   !Compute the local gfs:
   call dmft_gloc_matsubara(Ebethe,Dbethe,H0,Gmats,Smats)

   call dmft_self_consistency(Gmats(1,:,:,:,:,:,:),Gmats(2,:,:,:,:,:,:),&
        Smats(1,:,:,:,:,:,:),Smats(2,:,:,:,:,:,:),&
        Weiss(1,:,:,:,:,:,:),Weiss(2,:,:,:,:,:,:),&
        Hloc,trim(cg_scheme))
   call dmft_print_gf_matsubara(Gmats(1,:,:,:,:,:,:),"Gloc",iprint=1)
   call dmft_print_gf_matsubara(Gmats(2,:,:,:,:,:,:),"Floc",iprint=1)
   call dmft_print_gf_matsubara(Weiss(1,:,:,:,:,:,:),"Weiss",iprint=1)
   call dmft_print_gf_matsubara(Weiss(2,:,:,:,:,:,:),"fWeiss",iprint=1)
   !Perform the self-consistency fitting the new bath
   call ed_chi2_fitgf(Weiss,bath,ispin=1)
   !if it holds apply symmetrizations
   if(phsym)call ed_ph_symmetrize_bath(bath,save=.true.)
   if(normal_bath)call ed_enforce_normal_bath(bath,save=.true.)
   !MIXING:
   if(iloop>1)Bath = wmixing*Bath + (1.d0-wmixing)*Bath_prev
   Bath_prev=Bath
   !Check convergence (if required change chemical potential)
   converged = check_convergence(Weiss(1,1,1,1,1,:),dmft_error,nsuccess,nloop,reset=.false.)
   if(nread/=0.d0)call ed_search_variable(xmu,dens,converged)
   !Close this DMFT loop
   call end_loop
enddo
```

Printout GF and WF



ed_ahm_bethe.f90 solve the attractive Hubbard model on the be the Lattice

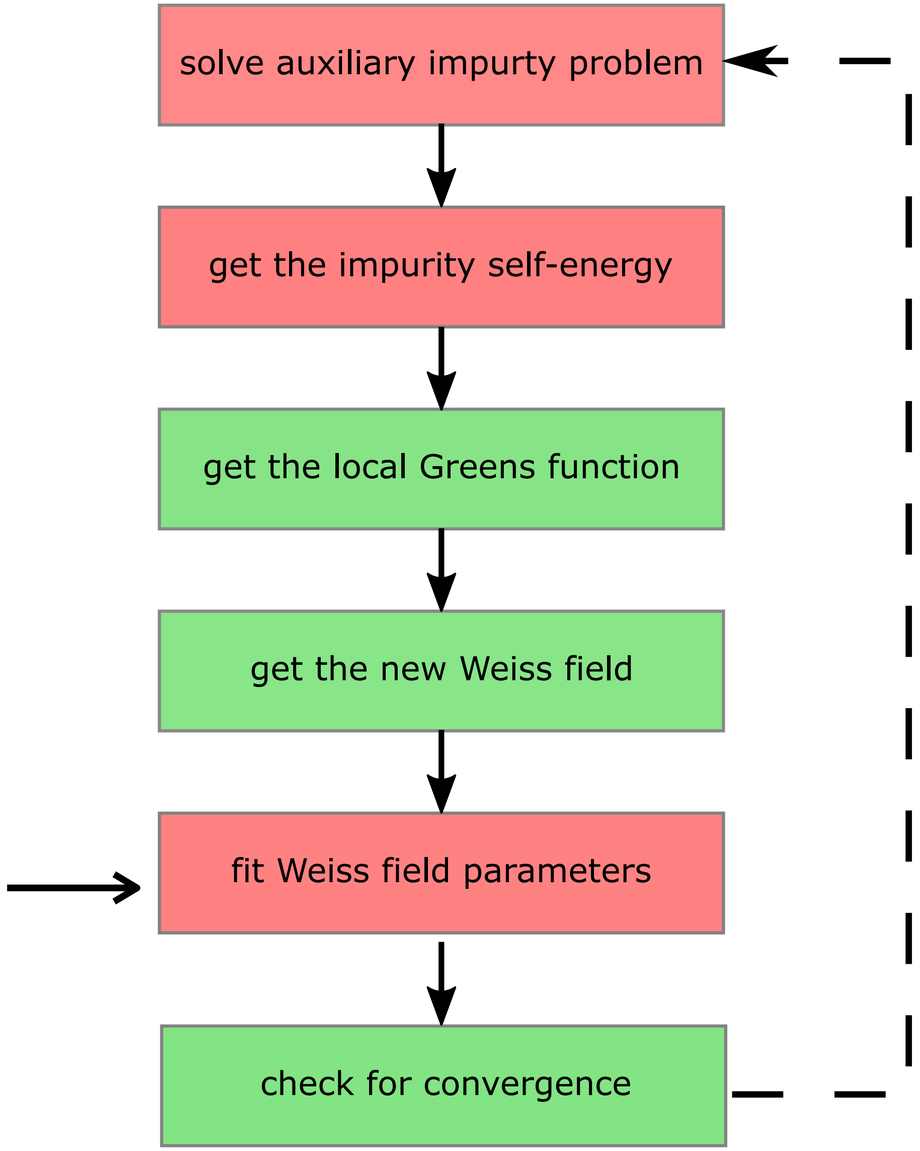
```
!DMFT loop
iloop=0;converged=.false.
do while(.not.converged.AND.iloop<nloop)
   iloop=iloop+1
   call start_loop(iloop,nloop,"DMFT-loop")
   !Solve the EFFECTIVE IMPURITY PROBLEM (first w/ a guess for the bath)
   call ed_solve(bath,Hloc)

   !Retrieve impurity self-energies (normal, anomalous)
   call ed_get_Sigma_matsubara(Smats(1,:,:,:,:,:,:))
   call ed_get_Self_matsubara(Smats(2,:,:,:,:,:,:))
   call ed_get_Sigma_realaxis(Sreal(1,:,:,:,:,:,:))
   call ed_get_Self_realaxis(Sreal(2,:,:,:,:,:,:))
   call ed_get_dens(dens,iorb=1)

   !Compute the local gfs:
   call dmft_gloc_matsubara(Ebethe,Dbethe,H0,Gmats,Smats)

   call dmft_self_consistency(Gmats(1,:,:,:,:,:,:),Gmats(2,:,:,:,:,:,:),&
        Smats(1,:,:,:,:,:,:),Smats(2,:,:,:,:,:,:),&
        Weiss(1,:,:,:,:,:,:),Weiss(2,:,:,:,:,:,:),&
        Hloc,trim(cg_scheme))
   call dmft_print_gf_matsubara(Gmats(1,:,:,:,:,:,:),"Gloc",iprint=1)
   call dmft_print_gf_matsubara(Gmats(2,:,:,:,:,:,:),"Floc",iprint=1)
   call dmft_print_gf_matsubara(Weiss(1,:,:,:,:,:,:),"Weiss",iprint=1)
   call dmft_print_gf_matsubara(Weiss(2,:,:,:,:,:,:),"fWeiss",iprint=1)
   !Perform the self-consistency fitting the new bath
   call ed_chi2_fitgf(Weiss,bath,ispin=1)
   !if it holds apply symmetrizations
   if(phsym)call ed_ph_symmetrize_bath(bath,save=.true.)
   if(normal_bath)call ed_enforce_normal_bath(bath,save=.true.)
   !MIXING:
   if(iloop>1)Bath = wmixing*Bath + (1.d0-wmixing)*Bath_prev
   Bath_prev=Bath
   !Check convergence (if required change chemical potential)
   converged = check_convergence(Weiss(1,1,1,1,1,:),dmft_error,nsuccess,nloop,reset=.false.)
   if(nread/=0.d0)call ed_search_variable(xmu,dens,converged)
   !Close this DMFT loop
   call end_loop
enddo
```

Get the new bath Parameters



ed_ahm_bethe.f90 solve the attractive Hubbard model on the be the Lattice

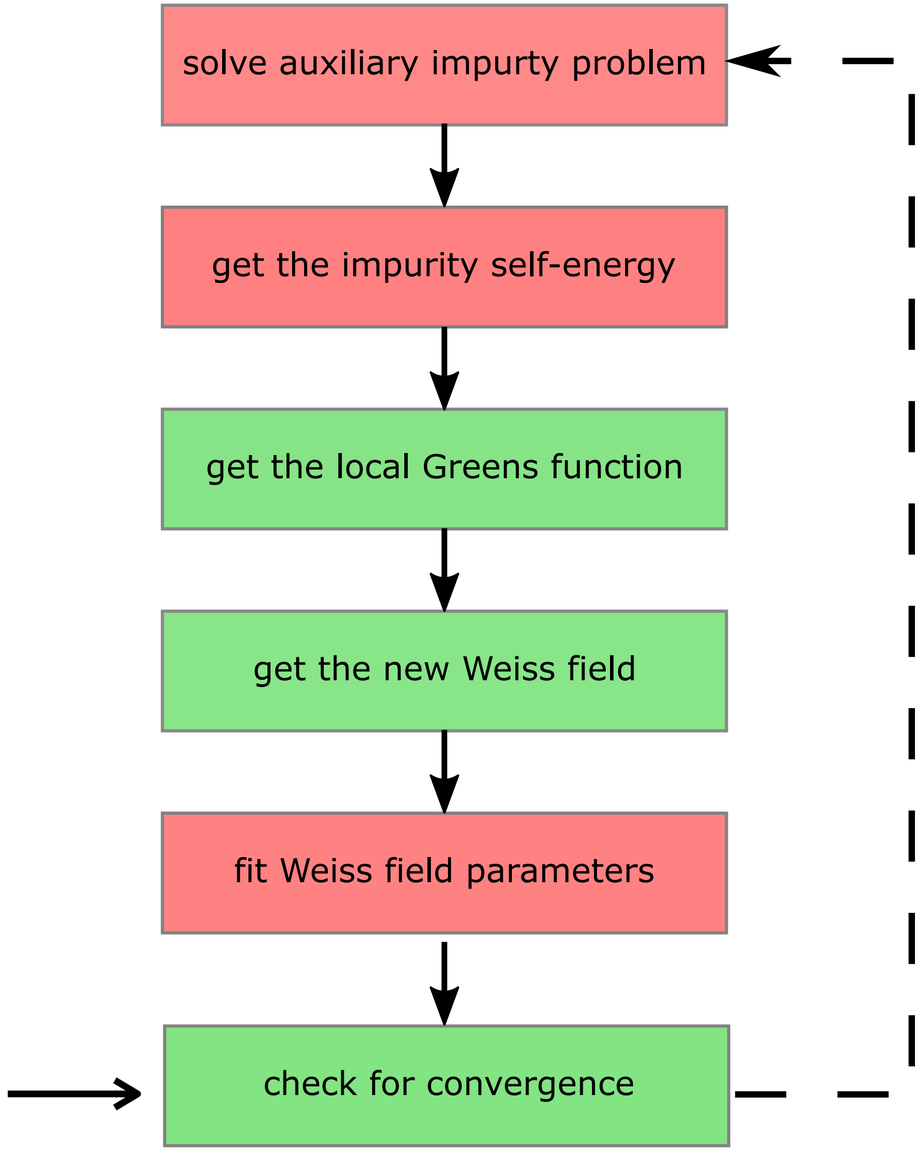
```
!DMFT loop
iloop=0;converged=.false.
do while(.not.converged.AND.iloop<nloop)
   iloop=iloop+1
   call start_loop(iloop,nloop,"DMFT-loop")
   !Solve the EFFECTIVE IMPURITY PROBLEM (first w/ a guess for the bath)
   call ed_solve(bath,Hloc)

   !Retrieve impurity self-energies (normal, anomalous)
   call ed_get_Sigma_matsubara(Smats(1,:,:,:,:,:,:))
   call ed_get_Self_matsubara(Smats(2,:,:,:,:,:,:))
   call ed_get_Sigma_realaxis(Sreal(1,:,:,:,:,:,:))
   call ed_get_Self_realaxis(Sreal(2,:,:,:,:,:,:))
   call ed_get_dens(dens,iorb=1)

   !Compute the local gfs:
   call dmft_gloc_matsubara(Ebethe,Dbethe,H0,Gmats,Smats)

   call dmft_self_consistency(Gmats(1,:,:,:,:,:,:),Gmats(2,:,:,:,:,:,:),&
        Smats(1,:,:,:,:,:,:),Smats(2,:,:,:,:,:,:),&
        Weiss(1,:,:,:,:,:,:),Weiss(2,:,:,:,:,:,:),&
        Hloc,trim(cg_scheme))
   call dmft_print_gf_matsubara(Gmats(1,:,:,:,:,:,:),"Gloc",iprint=1)
   call dmft_print_gf_matsubara(Gmats(2,:,:,:,:,:,:),"Floc",iprint=1)
   call dmft_print_gf_matsubara(Weiss(1,:,:,:,:,:,:),"Weiss",iprint=1)
   call dmft_print_gf_matsubara(Weiss(2,:,:,:,:,:,:),"fWeiss",iprint=1)
   !Perform the self-consistency fitting the new bath
   call ed_chi2_fitgf(Weiss,bath,ispin=1)
   !if it holds apply symmetrizations
   if(phsym)call ed_ph_symmetrize_bath(bath,save=.true.)
   if(normal_bath)call ed_enforce_normal_bath(bath,save=.true.)
   !MIXING:
   if(iloop>1)Bath = wmixing*Bath + (1.d0-wmixing)*Bath_prev
   Bath_prev=Bath
   !Check convergence (if required change chemical potential)
   converged = check_convergence(Weiss(1,1,1,1,1,:),dmft_error,nsuccess,nloop,reset=.false.)
   if(nread/=0.d0)call ed_search_variable(xmu,dens,converged)
   !Close this DMFT loop
   call end_loop
enddo
```

Convergence check

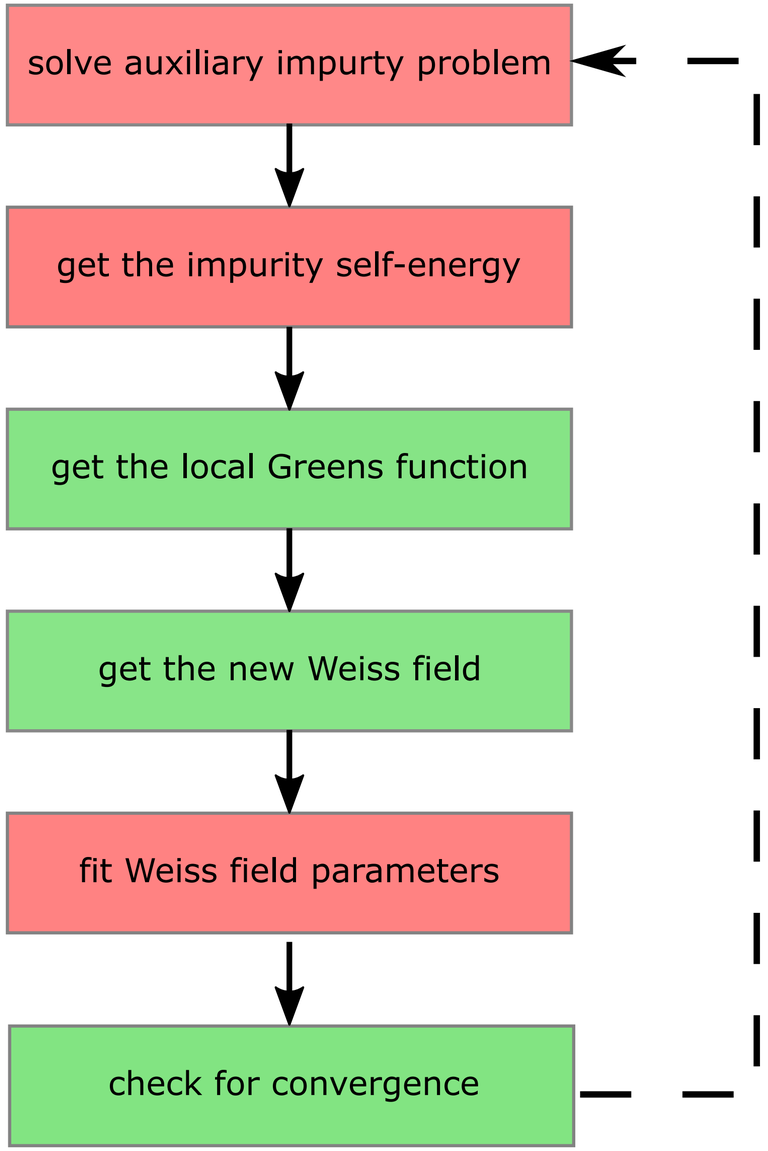


ed_ahm_bethe.f90 solve the attractive Hubbard model on the be the Lattice

```
   call end_loop
enddo
```

@convergence get GF in real frequency; Compute the kinetic energy

```
!Compute the local gfs:
call dmft_gloc_realaxis(Ebethe,Dbethe,H0,Greal,Sreal)
call dmft_print_gf_realaxis(Greal(1,:,:,:,:,:),"Gloc",iprint=1)
call dmft_print_gf_realaxis(Greal(2,:,:,:,:,:),"Floc",iprint=1)
!Compute the Kinetic Energy:
call dmft_kinetic_energy(Ebethe,Dbethe,H0,Smats(1,:,:,:,:,:),Smats(2,:,:,:,:,:))
!
```



```
WBAND=1.000000000                       !Bethe Lattice bandwidth
LE=1000                                 !Number of energy levels for Bethe DOS integration
WMIXING=7.500000000E-01                 !Mixing bath parameter
PHSYM=T                                 !Flag to enforce p-h symmetry of the bath.
NORMAL=F                                !Flag to enforce no symmetry braking in the bath.
NORB=1                                  !Number of impurity orbitals (max 5).
NBATH=6                                 !Number of bath sites:(normal=>Nbath per orb)(hybrid=>Nbath total)(replica=>Nbath=Nreplica)
NSPIN=1                                 !Number of spin degeneracy (max 2)
NPH=0                                   !Max number of phonons allowed (cut off)
BATH_TYPE=normal                        !flag to set bath type: normal (1bath/imp), hybrid(1bath), replica(1replica/imp)
ULOC=-2.050000000,0.d0,0.d0,0.d0,0.d0   !Values of the local interaction per orbital (max 5)
UST=0.d0                                !Value of the inter-orbital interaction term
JH=0.d0                                 !Hunds coupling
JX=0.d0                                 !S-E coupling
JP=0.d0                                 !P-H coupling
NLOOP=100                               !Max number of DMFT iterations.
NSUCCESS=1                              !Number of successive iterations below threshold for convergence
DMFT_ERROR=1.000000000E-05              !Error threshold for DMFT convergence
SB_FIELD=1.000000000E-01                !Value of a symmetry breaking field for magnetic solutions.
DELTASC=2.000000000E-02                 !Value of the SC symmetry breaking term.
BETA=1000.000000000                     !Inverse temperature, at T=0 is used as a IR cut-off.
XMU=0.d0                                !Chemical potential. If HFMODE=T, xmu=0 indicates half-filling condition.
G_PH=0.d0,0.d0,0.d0,0.d0,0.d0           !Electron-phonon coupling constant
W0_PH=0.d0                              !Phonon frequency
SPIN_FIELD_X=0.d0,0.d0,0.d0,0.d0,0.d0   !magnetic field per orbital coupling to X-spin component
SPIN_FIELD_Y=0.d0,0.d0,0.d0,0.d0,0.d0   !magnetic field per orbital coupling to Y-spin component
SPIN_FIELD_Z=0.d0,0.d0,0.d0,0.d0,0.d0   !magnetic field per orbital coupling to Z-spin component
EXC_FIELD=0.d0,0.d0,0.d0,0.d0           !external field coupling to exciton order parameters
PAIR_FIELD=0.d0,0.d0,0.d0,0.d0,0.d0     !pair field per orbital coupling to s-wave order parameter component
ED_MODE=superc                          !Flag to set ED type: normal=normal, superc=superconductive, nonsu2=broken SU(2)
ED_DIAG_TYPE=lanc                       !flag to select the diagonalization type: 'lanc' for Lanczos/Davidson, 'full' for Full diagonalization method
ED_FINITE_TEMP=F                        !flag to select finite temperature method. note that if T then lanc_nstates_total must be > 1
ED_TWIN=F                               !flag to reduce (T) or not (F,default) the number of visited sector using twin symmetry.
ED_SECTORS=F                            !flag to reduce sector scan for the spectrum to specific sectors +/- ed_sectors_shift.
ED_SECTORS_SHIFT=1                      !shift to ed_sectors
ED_SPARSE_H=T                           !flag to select  storage of sparse matrix H (mem--, cpu++) if TRUE, or direct on-the-fly H*v product (mem++, cpu--) if
ED_TOTAL_UD=T                           !flag to select which type of quantum numbers have to be considered: T (default) total Nup-Ndw, F orbital based Nup-Ndw
ED_SOLVE_OFFDIAG_GF=F                   !flag to select the calculation of the off-diagonal impurity GF. this is T by default if bath_type/=normal
ED_PRINT_SIGMA=T                        !flag to print impurity Self-energies
ED_PRINT_G=T                            !flag to print impurity Greens function
ED_PRINT_G0=T                           !flag to print non-interacting impurity Greens function
ED_ALL_G=T                              !flag to evaluate all the components of the impurity Green`s functions irrespective of the symmetries
ED_VERBOSE=3                            !Verbosity level: 0=almost nothing --> 5:all. Really: all
```

```
WBAND=1.000000000                       !Bethe Lattice bandwidth
LE=1000                                 !Number of energy levels for Bethe DOS integration
WMIXING=7.500000000E-01                 !Mixing bath parameter
PHSYM=T                                 !Flag to enforce p-h symmetry of the bath.
NORMAL=F                                !Flag to enforce no symmetry braking in the bath.
NORB=1                                  !Number of impurity orbitals (max 5).
NBATH=6                                 !Number of bath sites:(normal=>Nbath per orb)(hybrid=>Nbath total)(replica=>Nbath=Nreplica)
NSPIN=1                                 !Number of spin degeneracy (max 2)
NPH=0                                   !Max number of phonons allowed (cut off)
BATH_TYPE=normal                        !flag to set bath type: normal (1bath/imp), hybrid(1bath), replica(1replica/imp)
ULOC=-2.050000000,0.d0,0.d0,0.d0,0.d0   !Values of the local interaction per orbital (max 5)
UST=0.d0                                !Value of the inter-orbital interaction term
JH=0.d0                                 !Hunds coupling
JX=0.d0                                 !S-E coupling
JP=0.d0                                 !P-H coupling
NLOOP=100                               !Max number of DMFT iterations.
NSUCCESS=1                              !Number of successive iterations below threshold for convergence
DMFT_ERROR=1.000000000E-05              !Error threshold for DMFT convergence
SB_FIELD=1.000000000E-01                !Value of a symmetry breaking field for magnetic solutions.
DELTASC=2.000000000E-02                 !Value of the SC symmetry breaking term.
BETA=1000.000000000                     !Inverse temperature, at T=0 is used as a IR cut-off.
XMU=0.d0                                !Chemical potential. If HFMODE=T, xmu=0 indicates half-filling condition.
G_PH=0.d0,0.d0,0.d0,0.d0,0.d0           !Electron-phonon coupling constant
W0_PH=0.d0                              !Phonon frequency
SPIN_FIELD_X=0.d0,0.d0,0.d0,0.d0,0.d0   !magnetic field per orbital coupling to X-spin component
SPIN_FIELD_Y=0.d0,0.d0,0.d0,0.d0,0.d0   !magnetic field per orbital coupling to Y-spin component
SPIN_FIELD_Z=0.d0,0.d0,0.d0,0.d0,0.d0   !magnetic field per orbital coupling to Z-spin component
EXC_FIELD=0.d0,0.d0,0.d0,0.d0           !external field coupling to exciton order parameters
PAIR_FIELD=0.d0,0.d0,0.d0,0.d0,0.d0     !pair field per orbital coupling to s-wave order parameter component
```

MODEL AND PARAMETERS OF DMFT LOOP

```
ED_MODE=superc                          !Flag to set ED type: normal=normal, superc=superconductive, nonsu2=broken SU(2)
ED_DIAG_TYPE=lanc                       !flag to select the diagonalization type: 'lanc' for Lanczos/Davidson, 'full' for Full diagonalization method
ED_FINITE_TEMP=F                        !flag to select finite temperature method. note that if T then lanc_nstates_total must be > 1
ED_TWIN=F                               !flag to reduce (T) or not (F,default) the number of visited sector using twin symmetry.
ED_SECTORS=F                            !flag to reduce sector scan for the spectrum to specific sectors +/- ed_sectors_shift.
ED_SECTORS_SHIFT=1                      !shift to ed_sectors
ED_SPARSE_H=T                           !flag to select  storage of sparse matrix H (mem--, cpu++) if TRUE, or direct on-the-fly H*v product (mem++, cpu--) if
ED_TOTAL_UD=T                           !flag to select which type of quantum numbers have to be considered: T (default) total Nup-Ndw, F orbital based Nup-Ndw
ED_SOLVE_OFFDIAG_GF=F                   !flag to select the calculation of the off-diagonal impurity GF. this is T by default if bath_type/=normal
ED_PRINT_SIGMA=T                        !flag to print impurity Self-energies
ED_PRINT_G=T                            !flag to print impurity Greens function
ED_PRINT_G0=T                           !flag to print non-interacting impurity Greens function
ED_ALL_G=T                              !flag to evaluate all the components of the impurity Green`s functions irrespective of the symmetries
ED_VERBOSE=3                            !Verbosity level: 0=almost nothing --> 5:all. Really: all
```

```
WBAND=1.000000000                          !Bethe Lattice bandwidth
LE=1000                                    !Number of energy levels for Bethe DOS integration
WMIXING=7.500000000E-01                    !Mixing bath parameter
PHSYM=T                                    !Flag to enforce p-h symmetry of the bath.
NORMAL=F                                   !Flag to enforce no symmetry braking in the bath.
NORB=1                                     !Number of impurity orbitals (max 5).
NBATH=6                                    !Number of bath sites:(normal=>Nbath per orb)(hybrid=>Nbath total)(replica=>Nbath=Nreplica)
NSPIN=1                                    !Number of spin degeneracy (max 2)
NPH=0                                      !Max number of phonons allowed (cut off)
BATH_TYPE=normal                           !flag to set bath type: normal (1bath/imp), hybrid(1bath), replica(1replica/imp)
ULOC=-2.050000000,0.d0,0.d0,0.d0,0.d0      !Values of the local interaction per orbital (max 5)
UST=0.d0                                   !Value of the inter-orbital interaction term
JH=0.d0                                    !Hunds coupling
JX=0.d0                                    !S-E coupling
JP=0.d0                                    !P-H coupling
NLOOP=100                                  !Max number of DMFT iterations.
NSUCCESS=1                                 !Number of successive iterations below threshold for convergence
DMFT_ERROR=1.000000000E-05                 !Error threshold for DMFT convergence
SB_FIELD=1.000000000E-01                   !Value of a symmetry breaking field for magnetic solutions.
DELTASC=2.000000000E-02                    !Value of the SC symmetry breaking term.
BETA=1000.000000000                        !Inverse temperature, at T=0 is used as a IR cut-off.
XMU=0.d0                                   !Chemical potential. If HFMODE=T, xmu=0 indicates half-filling condition.
G_PH=0.d0,0.d0,0.d0,0.d0,0.d0              !Electron-phonon coupling constant
W0_PH=0.d0                                 !Phonon frequency
SPIN_FIELD_X=0.d0,0.d0,0.d0,0.d0,0.d0      !magnetic field per orbital coupling to X-spin component
SPIN_FIELD_Y=0.d0,0.d0,0.d0,0.d0,0.d0      !magnetic field per orbital coupling to Y-spin component
SPIN_FIELD_Z=0.d0,0.d0,0.d0,0.d0,0.d0      !magnetic field per orbital coupling to Z-spin component
EXC_FIELD=0.d0,0.d0,0.d0,0.d0              !external field coupling to exciton order parameters
PAIR_FIELD=0.d0,0.d0,0.d0,0.d0,0.d0        !pair field per orbital coupling to s-wave order parameter component
```

MODEL AND PARAMETERS OF DMFT LOOP

```
ED_MODE=superc                             !Flag to set ED type: normal=normal, superc=superconductive, nonsu2=broken SU(2)
ED_DIAG_TYPE=lanc                          !flag to select the diagonalization type: 'lanc' for Lanczos/Davidson, 'full' for Full diagonalization method
ED_FINITE_TEMP=F                           !flag to select finite temperature method. note that if T then lanc_nstates_total must be > 1
ED_TWIN=F                                  !flag to reduce (T) or not (F,default) the number of visited sector using twin symmetry.
ED_SECTORS=F                               !flag to reduce sector scan for the spectrum to specific sectors +/- ed_sectors_shift.
ED_SECTORS_SHIFT=1                         !shift to ed_sectors
ED_SPARSE_H=T                              !flag to select  storage of sparse matrix H (mem--, cpu++) if TRUE, or direct on-the-fly H*v product (mem++, cpu--) if
ED_TOTAL_UD=T                              !flag to select which type of quantum numbers have to be considered: T (default) total Nup-Ndw, F orbital based Nup-Nd
ED_SOLVE_OFFDIAG_GF=F                      !flag to select the calculation of the off-diagonal impurity GF. this is T by default if bath_type/=normal
ED_PRINT_SIGMA=T                           !flag to print impurity Self-energies
ED_PRINT_G=T                               !flag to print impurity Greens function
ED_PRINT_G0=T                              !flag to print non-interacting impurity Greens function
ED_ALL_G=T                                 !flag to evaluate all the components of the impurity Green`s functions irrespective of the symmetries
ED_VERBOSE=3                               !Verbosity level: 0=almost nothing --> 5:all. Really: all
```

ED-SOLVER

```
WBAND=1.000000000                       !Bethe Lattice bandwidth
LE=1000                                 !Number of energy levels for Bethe DOS integration
WMIXING=7.500000000E-01                 !Mixing bath parameter
PHSYM=T                                 !Flag to enforce p-h symmetry of the bath.
NORMAL=F                                !Flag to enforce no symmetry braking in the bath.
NORB=1                                  !Number of impurity orbitals (max 5).
NBATH=6                                 !Number of bath sites:(normal=>Nbath per orb)(hybrid=>Nbath total)(replica=>Nbath=Nreplica)
NSPIN=1                                 !Number of spin degeneracy (max 2)
NPH=0                                   !Max number of phonons allowed (cut off)
BATH_TYPE=normal                        !flag to set bath type: normal (1bath/imp), hybrid(1bath), replica(1replica/imp)
ULOC=-2.050000000,0.d0,0.d0,0.d0,0.d0   !Values of the local interaction per orbital (max 5)
UST=0.d0                                !Value of the inter-orbital interaction term
JH=0.d0                                 !Hunds coupling
JX=0.d0                                 !S-E coupling
JP=0.d0                                 !P-H coupling
NLOOP=100                               !Max number of DMFT iterations.
NSUCCESS=1                              !Number of successive iterations below threshold for convergence
DMFT_ERROR=1.000000000E-05              !Error threshold for DMFT convergence
SB_FIELD=1.000000000E-01                !Value of a symmetry breaking field for magnetic solutions.
DELTASC=2.000000000E-02                 !Value of the SC symmetry breaking term.
BETA=1000.000000000                     !Inverse temperature, at T=0 is used as a IR cut-off.
XMU=0.d0                                !Chemical potential. If HFMODE=T, xmu=0 indicates half-filling condition.
G_PH=0.d0,0.d0,0.d0,0.d0,0.d0           !Electron-phonon coupling constant
W0_PH=0.d0                              !Phonon frequency
SPIN_FIELD_X=0.d0,0.d0,0.d0,0.d0,0.d0   !magnetic field per orbital coupling to X-spin component
SPIN_FIELD_Y=0.d0,0.d0,0.d0,0.d0,0.d0   !magnetic field per orbital coupling to Y-spin component
SPIN_FIELD_Z=0.d0,0.d0,0.d0,0.d0,0.d0   !magnetic field per orbital coupling to Z-spin component
EXC_FIELD=0.d0,0.d0,0.d0,0.d0           !external field coupling to exciton order parameters
PAIR_FIELD=0.d0,0.d0,0.d0,0.d0,0.d0     !pair field per orbital coupling to s-wave order parameter component
ED_MODE=superc                          !Flag to set ED type: normal=normal, superc=superconductive, nonsu2=broken SU(2)
ED_DIAG_TYPE=lanc                       !flag to select the diagonalization type: 'lanc' for Lanczos/Davidson, 'f
ED_FINITE_TEMP=F                        !flag to select finite temperature method. note that if T then lanc_nstat
ED_TWIN=F                               !flag to reduce (T) or not (F,default) the number of visited sector using
ED_SECTORS=F                            !flag to reduce sector scan for the spectrum to specific sectors +/- ed_s
ED_SECTORS_SHIFT=1                      !shift to ed_sectors
ED_SPARSE_H=T                           !flag to select  storage of sparse matrix H (mem--, cpu++) if TRUE, or direct on-the-fly H*v product (mem++, cpu--) if
ED_TOTAL_UD=T                           !flag to select which type of quantum numbers have to be considered: T (default) total Nup-Ndw, F orbital based Nup-Ndw
ED_SOLVE_OFFDIAG_GF=F                   !flag to select the calculation of the off-diagonal impurity GF. this is T by default if bath_type/=normal
ED_PRINT_SIGMA=T                        !flag to print impurity Self-energies
ED_PRINT_G=T                            !flag to print impurity Greens function
ED_PRINT_G0=T                           !flag to print non-interacting impurity Greens function
ED_ALL_G=T                              !flag to evaluate all the components of the impurity Green`s functions irrespective of the symmetries
ED_VERBOSE=3                            !Verbosity level: 0=almost nothing --> 5:all. Really: all
```

driver

MODEL AND PARAMETERS OF DMFT LOOP

```
WBAND=1.000000000                          !Bethe Lattice bandwidth
LE=1000                                    !Number of energy levels for Bethe DOS integration
WMIXING=7.500000000E-01                    !Mixing bath parameter
PHSYM=T                                    !Flag to enforce p-h symmetry of the bath.
NORMAL=F                                   !Flag to enforce no symmetry braking in the bath.
NORB=1                                     !Number of impurity orbitals (max 5).
NBATH=6                                    !Number of bath sites:(normal=>Nbath per orb)(hybrid=>Nbath total)(replica=>Nbath=Nreplica)
NSPIN=1                                    !Number of spin degeneracy (max 2)
NPH=0                                      !Max number of phonons allowed (cut off)
BATH_TYPE=normal                           !flag to set bath type: normal (1bath/imp), hybrid(1bath), replica(1replica/imp)
ULOC=-2.050000000,0.d0,0.d0,0.d0,0.d0      !Values of the local interaction per orbital (max 5)
UST=0.d0                                   !Value of the inter-orbital interaction term
JH=0.d0                                    !Hunds coupling
JX=0.d0                                    !S-E coupling
JP=0.d0                                    !P-H coupling
NLOOP=100                                  !Max number of DMFT iterations.
NSUCCESS=1                                 !Number of successive iterations below threshold for convergence
DMFT_ERROR=1.000000000E-05                 !Error threshold for DMFT convergence
SB_FIELD=1.000000000E-01                   !Value of a symmetry breaking field for magnetic solutions.
DELTASC=2.000000000E-02                    !Value of the SC symmetry breaking term.
BETA=1000.000000000                        !Inverse temperature, at T=0 is used as a IR cut-off.
XMU=0.d0                                   !Chemical potential. If HFMODE=T, xmu=0 indicates half-filling condition.
G_PH=0.d0,0.d0,0.d0,0.d0,0.d0              !Electron-phonon coupling constant
W0_PH=0.d0                                 !Phonon frequency
SPIN_FIELD_X=0.d0,0.d0,0.d0,0.d0,0.d0      !magnetic field per orbital coupling to X-spin component
SPIN_FIELD_Y=0.d0,0.d0,0.d0,0.d0,0.d0      !magnetic field per orbital coupling to Y-spin component
SPIN_FIELD_Z=0.d0,0.d0,0.d0,0.d0,0.d0      !magnetic field per orbital coupling to Z-spin component
EXC_FIELD=0.d0,0.d0,0.d0,0.d0              !external field coupling to exciton order parameters
PAIR_FIELD=0.d0,0.d0,0.d0,0.d0,0.d0,0.d0   !pair field per orbital coupling to s-wave order parameter component
ED_MODE=superc                             !Flag to set ED type: normal=normal, superc=superconductive, nonsu2=broken SU(2)
ED_DIAG_TYPE=lanc                          !flag to select the diagonalization type: 'lanc' for Lanczos/Davidson, 'f
ED_FINITE_TEMP=F                           !flag to select finite temperature method. note that if T then lanc_nstat
ED_TWIN=F                                  !flag to reduce (T) or not (F,default) the number of visited sector using
ED_SECTORS=F                               !flag to reduce sector scan for the spectrum to specific sectors +/- ed_s
ED_SECTORS_SHIFT=1                         !shift to ed_sectors
ED_SPARSE_H=T                              !flag to select  storage of sparse matrix H (mem--, cpu++) if TRUE, or direct on-the-fly H*v product (mem++, cpu--) if
ED_TOTAL_UD=T                              !flag to select which type of quantum numbers have to be considered: T (default) total Nup-Ndw, F orbital based Nup-Ndw
ED_SOLVE_OFFDIAG_GF=F                      !flag to select the calculation of the off-diagonal impurity GF. this is T by default if bath_type/=normal
ED_PRINT_SIGMA=T                           !flag to print impurity Self-energies
ED_PRINT_G=T                               !flag to print impurity Greens function
ED_PRINT_G0=T                              !flag to print non-interacting impurity Greens function
ED_ALL_G=T                                 !flag to evaluate all the components of the impurity Green`s functions irrespective of the symmetries
ED_VERBOSE=3                               !Verbosity level: 0=almost nothing --> 5:all. Really: all
```

Number of orbitals
And number of sites in the bath

MODEL AND PARAMETERS OF DMFT LOOP

```
WBAND=1.000000000                          !Bethe Lattice bandwidth
LE=1000                                    !Number of energy levels for Bethe DOS integration
WMIXING=7.500000000E-01                    !Mixing bath parameter
PHSYM=T                                    !Flag to enforce p-h symmetry of the bath.
NORMAL=F                                   !Flag to enforce no symmetry braking in the bath.
NORB=1                                     !Number of impurity orbitals (max 5).
NBATH=6                                    !Number of bath sites:(normal=>Nbath per orb)(hybrid=>Nbath total)(replica=>Nbath=Nreplica)
NSPIN=1                                    !Number of spin degeneracy (max 2)
NPH=0                                      !Max number of phonons allowed (cut off)
BATH_TYPE=normal                           !flag to set bath type: normal (1bath/imp), hybrid(1bath), replica(1replica/imp)
ULOC=-2.050000000,0.d0,0.d0,0.d0,0.d0      !Values of the local interaction per orbital (max 5)
UST=0.d0                                   !Value of the inter-orbital interaction term
JH=0.d0                                    !Hunds coupling
JX=0.d0                                    !S-E coupling
JP=0.d0                                    !P-H coupling
NLOOP=100                                  !Max number of DMFT iterations.
NSUCCESS=1                                 !Number of successive iterations below threshold for convergence
DMFT_ERROR=1.000000000E-05                 !Error threshold for DMFT convergence
SB_FIELD=1.000000000E-01                   !Value of a symmetry breaking field for magnetic solutions.
DELTASC=2.000000000E-02                    !Value of the SC symmetry breaking term.
BETA=1000.000000000                        !Inverse temperature, at T=0 is used as a IR cut-off.
XMU=0.d0                                   !Chemical potential. If HFMODE=T, xmu=0 indicates half-filling condition.
G_PH=0.d0,0.d0,0.d0,0.d0,0.d0              !Electron-phonon coupling constant
W0_PH=0.d0                                 !Phonon frequency
SPIN_FIELD_X=0.d0,0.d0,0.d0,0.d0,0.d0      !magnetic field per orbital coupling to X-spin component
SPIN_FIELD_Y=0.d0,0.d0,0.d0,0.d0,0.d0      !magnetic field per orbital coupling to Y-spin component
SPIN_FIELD_Z=0.d0,0.d0,0.d0,0.d0,0.d0      !magnetic field per orbital coupling to Z-spin component
EXC_FIELD=0.d0,0.d0,0.d0,0.d0              !external field coupling to exciton order parameters
PAIR_FIELD=0.d0,0.d0,0.d0,0.d0,0.d0,0.d0   !pair field per orbital coupling to s-wave order parameter component
ED_MODE=superc                             !Flag to set ED type: normal=normal, superc=superconductive, nonsu2=broken SU(2)
ED_DIAG_TYPE=lanc                          !flag to select the diagonalization type: 'lanc' for Lanczos/Davidson, 'f
ED_FINITE_TEMP=F                           !flag to select finite temperature method. note that if T then lanc_nstat
ED_TWIN=F                                  !flag to reduce (T) or not (F,default) the number of visited sector using
ED_SECTORS=F                               !flag to reduce sector scan for the spectrum to specific sectors +/- ed_s
ED_SECTORS_SHIFT=1                         !shift to ed_sectors
ED_SPARSE_H=T                              !flag to select  storage of sparse matrix H (mem--, cpu++) if TRUE, or direct on-the-fly H*v product (mem++, cpu--) if
ED_TOTAL_UD=T                              !flag to select which type of quantum numbers have to be considered: T (default) total Nup-Ndw, F orbital based Nup-Ndw
ED_SOLVE_OFFDIAG_GF=F                      !flag to select the calculation of the off-diagonal impurity GF. this is T by default if bath_type/=normal
ED_PRINT_SIGMA=T                           !flag to print impurity Self-energies
ED_PRINT_G=T                               !flag to print impurity Greens function
ED_PRINT_G0=T                              !flag to print non-interacting impurity Greens function
ED_ALL_G=T                                 !flag to evaluate all the components of the impurity Green`s functions irrespective of the symmetries
ED_VERBOSE=3                               !Verbosity level: 0=almost nothing --> 5:all. Really: all
```

Interaction Hamiltonian

MODEL AND PARAMETERS OF DMFT LOOP

```
WBAND=1.000000000                          !Bethe Lattice bandwidth
LE=1000                                    !Number of energy levels for Bethe DOS integration
WMIXING=7.500000000E-01                    !Mixing bath parameter
PHSYM=T                                    !Flag to enforce p-h symmetry of the bath.
NORMAL=F                                   !Flag to enforce no symmetry braking in the bath.
NORB=1                                     !Number of impurity orbitals (max 5).
NBATH=6                                    !Number of bath sites:(normal=>Nbath per orb)(hybrid=>Nbath total)(replica=>Nbath=Nreplica)
NSPIN=1                                    !Number of spin degeneracy (max 2)
NPH=0                                      !Max number of phonons allowed (cut off)
BATH_TYPE=normal                           !flag to set bath type: normal (1bath/imp), hybrid(1bath), replica(1replica/imp)
ULOC=-2.050000000,0.d0,0.d0,0.d0,0.d0      !Values of the local interaction per orbital (max 5)
UST=0.d0                                   !Value of the inter-orbital interaction term
JH=0.d0                                    !Hunds coupling
JX=0.d0                                    !S-E coupling
JP=0.d0                                    !P-H coupling
NLOOP=100                                  !Max number of DMFT iterations.
NSUCCESS=1                                 !Number of successive iterations below threshold for convergence
DMFT_ERROR=1.000000000E-05                 !Error threshold for DMFT convergence
SB_FIELD=1.000000000E-01                   !Value of a symmetry breaking field for magnetic solutions.
DELTASC=2.000000000E-02                    !Value of the SC symmetry breaking term.
BETA=1000.000000000                        !Inverse temperature, at T=0 is used as a IR cut-off.
XMU=0.d0                                   !Chemical potential. If HFMODE=T, xmu=0 indicates half-filling condition.
G_PH=0.d0,0.d0,0.d0,0.d0,0.d0              !Electron-phonon coupling constant
W0_PH=0.d0                                 !Phonon frequency
SPIN_FIELD_X=0.d0,0.d0,0.d0,0.d0,0.d0      !magnetic field per orbital coupling to X-spin component
SPIN_FIELD_Y=0.d0,0.d0,0.d0,0.d0,0.d0      !magnetic field per orbital coupling to Y-spin component
SPIN_FIELD_Z=0.d0,0.d0,0.d0,0.d0,0.d0      !magnetic field per orbital coupling to Z-spin component
EXC_FIELD=0.d0,0.d0,0.d0,0.d0              !external field coupling to exciton order parameters
PAIR_FIELD=0.d0,0.d0,0.d0,0.d0,0.d0,0.d0   !pair field per orbital coupling to s-wave order parameter component
ED_MODE=superc                             !Flag to set ED type: normal=normal, superc=superconductive, nonsu2=broken SU(2)
ED_DIAG_TYPE=lanc                          !flag to select the diagonalization type: 'lanc' for Lanczos/Davidson, 'f
ED_FINITE_TEMP=F                           !flag to select finite temperature method. note that if T then lanc_nstat
ED_TWIN=F                                  !flag to reduce (T) or not (F,default) the number of visited sector using
ED_SECTORS=F                               !flag to reduce sector scan for the spectrum to specific sectors +/- ed_s
ED_SECTORS_SHIFT=1                         !shift to ed_sectors
ED_SPARSE_H=T                              !flag to select  storage of sparse matrix H (mem--, cpu++) if TRUE, or direct on-the-fly H*v product (mem++, cpu--) if
ED_TOTAL_UD=T                              !flag to select which type of quantum numbers have to be considered: T (default) total Nup-Ndw, F orbital based Nup-Ndw
ED_SOLVE_OFFDIAG_GF=F                      !flag to select the calculation of the off-diagonal impurity GF. this is T by default if bath_type/=normal
ED_PRINT_SIGMA=T                           !flag to print impurity Self-energies
ED_PRINT_G=T                               !flag to print impurity Greens function
ED_PRINT_G0=T                              !flag to print non-interacting impurity Greens function
ED_ALL_G=T                                 !flag to evaluate all the components of the impurity Green`s functions irrespective of the symmetries
ED_VERBOSE=3                               !Verbosity level: 0=almost nothing --> 5:all. Really: all
```

Error in DFMT loops

MODEL AND PARAMETERS OF DMFT LOOP

```
WBAND=1.000000000                       !Bethe Lattice bandwidth
LE=1000                                 !Number of energy levels for Bethe DOS integration
WMIXING=7.500000000E-01                 !Mixing bath parameter
PHSYM=T                                 !Flag to enforce p-h symmetry of the bath.
NORMAL=F                                !Flag to enforce no symmetry braking in the bath.
NORB=1                                  !Number of impurity orbitals (max 5).
NBATH=6                                 !Number of bath sites:(normal=>Nbath per orb)(hybrid=>Nbath total)(replica=>Nbath=Nreplica)
NSPIN=1                                 !Number of spin degeneracy (max 2)
NPH=0                                   !Max number of phonons allowed (cut off)
BATH_TYPE=normal                        !flag to set bath type: normal (1bath/imp), hybrid(1bath), replica(1replica/imp)
ULOC=-2.050000000,0.d0,0.d0,0.d0,0.d0   !Values of the local interaction per orbital (max 5)
UST=0.d0                                !Value of the inter-orbital interaction term
JH=0.d0                                 !Hunds coupling
JX=0.d0                                 !S-E coupling
JP=0.d0                                 !P-H coupling
NLOOP=100                               !Max number of DMFT iterations.
NSUCCESS=1                              !Number of successive iterations below threshold for convergence
DMFT_ERROR=1.000000000E-05              !Error threshold for DMFT convergence
SB_FIELD=1.000000000E-01                !Value of a symmetry breaking field for magnetic solutions.
DELTASC=2.000000000E-02                 !Value of the SC symmetry breaking term.
BETA=1000.000000000                     !Inverse temperature, at T=0 is used as a IR cut-off.
XMU=0.d0                                !Chemical potential. If HFMODE=T, xmu=0 indicates half-filling condition.
G_PH=0.d0,0.d0,0.d0,0.d0,0.d0           !Electron-phonon coupling constant
W0_PH=0.d0                              !Phonon frequency
SPIN_FIELD_X=0.d0,0.d0,0.d0,0.d0,0.d0   !magnetic field per orbital coupling to X-spin component
SPIN_FIELD_Y=0.d0,0.d0,0.d0,0.d0,0.d0   !magnetic field per orbital coupling to Y-spin component
SPIN_FIELD_Z=0.d0,0.d0,0.d0,0.d0,0.d0   !magnetic field per orbital coupling to Z-spin component
EXC_FIELD=0.d0,0.d0,0.d0,0.d0           !external field coupling to exciton order parameters
PAIR_FIELD=0.d0,0.d0,0.d0,0.d0,0.d0,0.d0 !pair field per orbital coupling to s-wave order parameter component
ED_MODE=superc                          !Flag to set ED type: normal=normal, superc=superconductive, nonsu2=broken SU(2)
ED_DIAG_TYPE=lanc                       !flag to select the diagonalization type: 'lanc' for Lanczos/Davidson, 'f
ED_FINITE_TEMP=F                        !flag to select finite temperature method. note that if T then lanc_nstat
ED_TWIN=F                               !flag to reduce (T) or not (F,default) the number of visited sector using
ED_SECTORS=F                            !flag to reduce sector scan for the spectrum to specific sectors +/- ed_s
ED_SECTORS_SHIFT=1                      !shift to ed_sectors
```

Temperature(*)
chemical potential
symmetry breaking fields

MODEL AND PARAMETERS OF
DMFT LOOP

(*) Temperature: here Temperature is just an IR cut-off for smooth fermi functions; See below for ACTUAL FINITE T calculations

ED_MODE = super/normal

ED_FINITE_TEMP =F/T

```
BETA=1000.000000000                !Inverse temperature, at T=0 is used as a IR cut-off.
XMU=0.d0                           !Chemical potential. If HFMODE=T, xmu=0 indicates half-filling condition.
G_PH=0.d0,0.d0,0.d0,0.d0,0.d0      !Electron-phonon coupling constant
W0_PH=0.d0                         !Phonon frequency
SPIN_FIELD_X=0.d0,0.d0,0.d0,0.d0,0.d0  !magnetic field per orbital coupling to X-spin component
SPIN_FIELD_Y=0.d0,0.d0,0.d0,0.d0,0.d0  !magnetic field per orbital coupling to Y-spin component
SPIN_FIELD_Z=0.d0,0.d0,0.d0,0.d0,0.d0  !magnetic field per orbital coupling to Z-spin component
EXC_FIELD=0.d0,0.d0,0.d0,0.d0      !external field coupling to exciton order parameters
PAIR_FIELD=0.d0,0.d0,0.d0,0.d0,0.d0  !pair field per orbital coupling to s-wave order parameter component
ED_MODE=superc                     !Flag to set ED type: normal=normal, superc=superconductive, nonsu2=broken SU(2)
ED_DIAG_TYPE=lanc                  !flag to select the diagonalization type: 'lanc' for Lanczos/Davidson, 'full' for Full diagonalization method
ED_FINITE_TEMP=F                   !flag to select finite temperature method. note that if T then lanc_nstates_total must be > 1
ED_TWIN=F                          !flag to reduce (T) or not (F,default) the number of visited sector using twin symmetry.
ED_SECTORS=F                       !flag to reduce sector scan for the spectrum to specific sectors +/- ed_sectors_shift.
ED_SECTORS_SHIFT=1                 !shift to ed_sectors
ED_SPARSE_H=T                      !flag to select  storage of sparse matrix H (mem--, cpu++) if TRUE, or direct on-the-fly H*v product (mem++, cpu--) if FALSE
ED_TOTAL_UD=T                      !flag to select which type of quantum numbers have to be considered: T (default) total Nup-Ndw, F orbital based Nup-Ndw
ED_SOLVE_OFFDIAG_GF=F              !flag to select the calculation of the off-diagonal impurity GF. this is T by default if bath_type/=normal
ED_PRINT_SIGMA=T                   !flag to print impurity Self-energies
ED_PRINT_G=T                       !flag to print impurity Greens function
ED_PRINT_G0=T                      !flag to print non-interacting impurity Greens function
ED_ALL_G=T                         !flag to evaluate all the components of the impurity Green`s functions irrespective of the symmetries
ED_VERBOSE=3                       !Verbosity level: 0=almost nothing --> 5:all. Really: all
ED_HW_BATH=2.000000000             !half-bandwidth for the bath initialization: flat in -hwband:hwband
ED_OFFSET_BATH=1.000000000E-01     !offset for the initialization of diagonal terms in replica bath: -offset:offset
LMATS=4096                         !Number of Matsubara frequencies.
LREAL=5000                         !Number of real-axis frequencies.
LTAU=1024                          !Number of imaginary time points.
LFIT=1000                          !Number of Matsubara frequencies used in the \Chi2 fit.
LPOS=100                           !Number of points for the lattice PDF.
```

```
CHIPAIR_FLAG=F                          !Flag to activate pair susceptibility calculation.
CHIEXCT_FLAG=F                          !Flag to activate excitonis susceptibility calculation.
HFMODE=T                                !Flag to set the Hartree form of the interaction (n-1/2). see xmu.
EPS=1.000000000E-02                     !Broadening on the real-axis.
CUTOFF=1.000000000E-09                  !Spectrum cut-off, used to determine the number states to be retained.
GS_THRESHOLD=1.000000000E-09             !Energy threshold for ground state degeneracy loop up
LANC_METHOD=arpack                      !select the lanczos method to be used in the determination of the spectrum  ARPACK (default), LANCZOS (T=0 only), DVDSON (no M
LANC_NSTATES_SECTOR=1                   !Initial number of states per sector to be determined.
LANC_NSTATES_TOTAL=1                    !Initial number of total states to be determined.
LANC_NSTATES_STEP=2                     !Number of states added to the spectrum at each step.
LANC_NCV_FACTOR=10                      !Set the size of the block used in Lanczos-Arpack by multiplying the required Neigen (Ncv=lanc_ncv_factor*Neigen+lanc_ncv_add)
LANC_NCV_ADD=0                          !Adds up to the size of the block to prevent it to become too small (Ncv=lanc_ncv_factor*Neigen+lanc_ncv_add)
LANC_NITER=1024                         !Number of Lanczos iteration in spectrum determination.
LANC_NGFITER=400                        !Number of Lanczos iteration in GF determination. Number of momenta.
LANC_TOLERANCE=1.000000000E-18          !Tolerance for the Lanczos iterations as used in Arpack and plain lanczos.
LANC_DIM_THRESHOLD=1024                 !Min dimension threshold to use Lanczos determination of the spectrum rather than Lapack based exact diagonalization.
CG_METHOD=1                             !Conjugate-Gradient method: 0=NR, 1=minimize.
CG_GRAD=0                               !Gradient evaluation method: 0=analytic (default), 1=numeric.
CG_FTOL=1.000000000E-05                 !Conjugate-Gradient tolerance.
CG_STOP=0                               !Conjugate-Gradient stopping condition: 0-3, 0=C1.AND.C2, 1=C1, 2=C2 with C1=|F_n-1 -F_n|<tol*(1+F_n), C2=||x_n-1 -x_n||<tol*(
x_n||).
CG_NITER=500                            !Max. number of Conjugate-Gradient iterations.
CG_WEIGHT=1                             !Conjugate-Gradient weight form: 1=1.0, 2=1/n , 3=1/w_n.
CG_SCHEME=delta                         !Conjugate-Gradient fit scheme: delta or weiss.
CG_POW=2                                !Fit power for the calculation of the Chi distance function as 1/L*|G0 - G0and|**cg_pow
CG_MINIMIZE_VER=F                       !Flag to pick old/.false. (Krauth) or new/.true. (Lichtenstein) version of the minimize CG routine
CG_MINIMIZE_HH=1.000000000E-04          !Unknown parameter used in the CG minimize procedure.
JZ_BASIS=F                              !
JZ_MAX=F                                !
```

```
CHIPAIR_FLAG=F                          !Flag to activate pair susceptibility calculation.
CHIEXCT_FLAG=F                          !Flag to activate excitonis susceptibility calculation.
HFMODE=T                                !Flag to set the Hartree form of the interaction (n-1/2). see xmu.
EPS=1.000000000E-02                     !Broadening on the real-axis.
CUTOFF=1.000000000E-09                  !Spectrum cut-off, used to determine the number states to be retained.
GS_THRESHOLD=1.000000000E-09            !Energy threshold for ground state degeneracy loop up
LANC_METHOD=arpack                      !select the lanczos method to be used in the determination of the spectrum. ARPACK (default), LANCZOS (T=0 only), DVDSON (no M
LANC_NSTATES_SECTOR=1                   !Initial number of states per sector to be determined.
LANC_NSTATES_TOTAL=1                    !Initial number of total states to be determined.
LANC_NSTATES_STEP=2                     !Number of states added to the spectrum at each step.
LANC_NCV_FACTOR=10                      !Set the size of the block used in Lanczos-Arpack by multiplying the required Neigen (Ncv=lanc_ncv_factor*Neigen+lanc_ncv_add)
LANC_NCV_ADD=0                          !Adds up to the size of the block to prevent it to become too small (Ncv=lanc_ncv_factor*Neigen+lanc_ncv_add)
LANC_NITER=1024                         !Number of Lanczos iteration in spectrum determination.
LANC_NGFITER=400                        !Number of Lanczos iteration in GF determination. Number of momenta.
LANC_TOLERANCE=1.000000000E-18          !Tolerance for the Lanczos iterations as used in Arpack and plain lanczos.
LANC_DIM_THRESHOLD=1024                 !Min dimension threshold to use Lanczos determination of the spectrum rather than Lapack based exact diagonalization.
CG_METHOD=1                             !Conjugate-Gradient method: 0=NR, 1=minimize.
CG_GRAD=0                               !Gradient evaluation method: 0=analytic (default), 1=numeric.
CG_FTOL=1.000000000E-05                 !Conjugate-Gradient tolerance.
CG_STOP=0                               !Conjugate-Gradient stopping condition: 0-3, 0=C1.AND.C2, 1=C1, 2=C2 with C1=|F_n-1 -F_n|<tol*(1+F_n), C2=||x_n-1 -x_n||<tol*(
x_n||).
CG_NITER=500                            !Max. number of Conjugate-Gradient iterations.
CG_WEIGHT=1                             !Conjugate-Gradient weight form: 1=1.0, 2=1/n , 3=1/w_n.
CG_SCHEME=delta                         !Conjugate-Gradient fit scheme: delta or weiss.
CG_POW=2                                !Fit power for the calculation of the Chi distance function as 1/L*|G0 - G0and|**cg_pow
CG_MINIMIZE_VER=F                       !Flag to pick old/.false. (Krauth) or new/.true. (Lichtenstein) version of the minimize CG routine
CG_MINIMIZE_HH=1.000000000E-04          !Unknown parameter used in the CG minimize procedure.
JZ_BASIS=F                              !
JZ_MAX=F                                !
```

FIT OF BATH PARAMETERS

In the DATA/init_run/ directory

```
[giacomo@hyperion 15:28 init_run (master)]$ ls -1
hamiltonian.restart
inputAHM.conf
run.sh
```

A reasonable guess for the parameters in the impurity hamiltonian

Input file

Bash script to run the code recursively

$$H_{imp}^{SC} = U n_{i\uparrow} n_{i\downarrow} - \mu \sum_{\sigma} n_{i\sigma} + \sum_{l\sigma} v_l c_{i\sigma}^{\dagger} d_{l\sigma} + h.c. + \sum_{l} \varepsilon_l d_{l\sigma}^{\dagger} d_{l\sigma} + \sum_{l} \Delta_l d_{l\uparrow}^{\dagger} d_{l\downarrow}^{\dagger} + h.c$$

```
[giacomo@hyperion 15:31 init_run (master)]$ cat hamiltonian.restart
            #Ek_l1_s1                  Dk_l1_s1                  Vk_l1_s1
  -7.350264028261E-01   -1.165133274030E+00   -2.605904767951E-01
  -4.082465585322E-01   -3.651036562198E-01    1.500611517845E-01
  -5.539808117348E-02   -5.612699572416E-01    1.850262221085E-01
   5.539808117348E-02   -5.612699572416E-01    1.850262221085E-01
   4.082465585322E-01   -3.651036562198E-01    1.500611517845E-01
   7.350264028261E-01   -1.165133274030E+00   -2.605904767951E-01
[giacomo@hyperion 15:31 init_run (master)]$
```

Run a single DMFT loop, ie Nloop=1 and read the output

```
INIT SOLVER FOR
Summary:
-----------------------------------------
# of levels/spin      =              7
Total size            =             14
# of impurities       =              1
# of bath/impurity    =              6
# of Bath levels/spin =              6
# of  sectors         =             15
Ns_Orb                =              7
Ns_Ud                 =              1
Nph                   =              0
Largest Sector(s)     =           3432
-----------------------------------------
```

Initialize the bath

```
-----DMFT-loop    1 (max:  100)-----
(  0.0000,  0.0000)

           #Ek_l1_s1              Dk_l1_s1              Vk_l1_s1
  -7.350264028261E-01   -1.165133274030E+00   -2.605904767951E-01
  -4.082465585322E-01   -3.651036562198E-01    1.500611517845E-01
  -5.539808117348E-02   -5.612699572416E-01    1.850262221085E-01
   5.539808117348E-02   -5.612699572416E-01    1.850262221085E-01
   4.082465585322E-01   -3.651036562198E-01    1.500611517845E-01
   7.350264028261E-01   -1.165133274030E+00   -2.605904767951E-01
Diagonalize impurity problem:
Diagonalize impurity H:
        1-Solving sector:        1   sz:  -7  dim=                  1
Total time [h:m:s.ms]:   0:00:00.000

        2-Solving sector:        2   sz:  -6  dim=                 14
Total time [h:m:s.ms]:   0:00:00.000

        3-Solving sector:        3   sz:  -5  dim=                 91
Total time [h:m:s.ms]:   0:00:00.002

        4-Solving sector:        4   sz:  -4  dim=                364
Total time [h:m:s.ms]:   0:00:00.072
```

start the diagonalization

```
Total time [h:m:s.ms]:   0:00:03.390
# i       E_i           exp(-(E-E0)/T)       Sz     Sect     Dim
     1   -5.720735175477   1.000000000000E+00   0      8      3432
Egs =     -5.720735175477   0
Z   =      1.000000000000
Get impurity Greens functions:
Get G&F_l1_s1
From sector  :     8     0
        apply c^+_a,up:  1
          apply c_a,up: -1
          apply c_a,dw:  1
        apply c^+_a,dw: -1
apply c^+_a,up + c_a,dw  1
apply c_a,up + c^+_a,dw -1
Total time [h:m:s.ms]:   0:00:00.511
Get observables:
dens=    1.000000000000    1.000000000000
docc=    0.442171769401
phi =   -0.426362048662   -0.852724097325
Get local energy:
<Hint>  =   -0.384343538802
<V>     =   -0.884343538802
<E0>    =    0.000000000000
<Ehf>   =    0.500000000000
Dust    =    0.000000000000
Dund    =    0.000000000000
Dse     =    0.000000000000
Dph     =    0.000000000000
```

end of the diagonalization

use LANCZOS to compute GF

$\langle n_i \rangle$

$\langle n_{i\uparrow} n_{i\downarrow} \rangle$

$\langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \rangle$

energy $\langle H_{int} \rangle$

obsevables

```
Get local Matsubara Superc Green's function (no print)

  +ETA --> fort.6
  10% |ETA: 0:00:03.965 @21 November 2021  22:36:10
  20% |ETA: 0:00:03.853
  30% |ETA: 0:00:03.832                          get local GF
  40% |ETA: 0:00:02.726
  50% |ETA: 0:00:02.595 @21 November 2021  22:36:11
  60% |ETA: 0:00:01.944
  70% |ETA: 0:00:01.702
  80% |ETA: 0:00:00.952
  90% |ETA: 0:00:00.951
 100% |ETA: 0:00:00.000                                  print local GF/WF/Sigma
Total time [h:m:s.ms]:   0:00:04.770
Gloc dmft_gfio: write spin-orbital diagonal elements.
Floc dmft_gfio: write spin-orbital diagonal elements.
Weiss dmft_gfio: write spin-orbital diagonal elements.
fWeiss dmft_gfio: write spin-orbital diagonal elements.
\Chi2 fit with CG-minimize and CG-weight: 1 on: delta        FIT
chi^2|iter=   5.428583883E-08 |    18  <--  Orb1 Spin1
            #Ek_l1_s1               Dk_l1_s1               Vk_l1_s1
  -7.368862472260E-01   -1.163963969987E+00   -2.549103937907E-01
  -4.106578097561E-01   -3.644053221024E-01    1.580654889513E-01
  -5.575033227078E-02   -5.603308273612E-01    1.863142740882E-01
   5.570751126489E-02   -5.603379748694E-01    1.862918353871E-01
   4.106364322785E-01   -3.644328121463E-01    1.579171693689E-01
   7.368634304659E-01   -1.163974976009E+00   -2.548497602797E-01
^[[1;91merror=^[[0m  1.0000000E+00    new bath parameters  after fit
====================================
Total time [h:m:s.ms]:   0:00:08.910      END of the dmft loop
```

release Nloop=1 and
bring the DMFT loop at convergence

output of files

```
[giacomo@work-laptop 15:34 uloc-2.00 (master)]$ ls
Floc_l11_s1_iw.dat          eigenvalues_list.ed       impF0_l11_s1_realw.ed     inputAHM.conf
Floc_l11_s1_realw.dat       energy_info.ed            impF_l11_s1_iw.ed         observables_all.ed
Gloc_l11_s1_iw.dat          energy_last.ed            impF_l11_s1_realw.ed      observables_info.ed
Gloc_l11_s1_realw.dat       error.err                 impG0_l11_s1_iw.ed        observables_last.ed
Hseed                       fWeiss_l11_s1_iw.dat      impG0_l11_s1_realw.ed     parameters_info.ed
LOG.file                    fit_delta_l1_s1.ed        impG_l11_s1_iw.ed         parameters_last.ed
Weiss_l11_s1_iw.dat         fit_fdelta_l1_s1.ed       impG_l11_s1_realw.ed      scifor_version.inc
chi2fit_results_orb1_s1.ed  gfmatrix.restart          impSelf_l11_s1_iw.ed      sectors.restart
code_version.inc            hamiltonian.restart       impSelf_l11_s1_realw.ed   state_list.ed
dmft_kinetic_energy.dat     hamiltonian.used          impSigma_l11_s1_iw.ed     used.inputAHM.conf
dmft_kinetic_energy.info    impF0_l11_s1_iw.ed        impSigma_l11_s1_realw.ed
[giacomo@work-laptop 15:34 uloc-2.00 (master)]$
```

ex: local observables

$ cat observables_info.ed

```
[giacomo@work-laptop 16:09 uloc-2.00 (master)]$ cat observables_info.ed
#   1dens_1          2phi_1          3docc_1          4nup_1          5ndw_1          6mag_1          7s2          8egs
    9sz2_11         10n2_11         11z_1s1       13sig_1s1
```

$ cat observables_all.ed

```
[giacomo@work-laptop 16:10 uloc-2.00 (master)]$
[giacomo@work-laptop 16:10 uloc-2.00 (master)]$ cat observables_all.ed
   1.000000000    -0.426362049     0.442171769     0.500000000     0.500000000    -0.000000000     0.028914115    -5.720735175
   0.028914115     1.884343539     0.848682115    -0.000000065
   1.000000000    -0.424653041     0.441228190     0.500000000     0.500000000     0.000000000     0.029385905    -5.723766751
   0.029385905     1.882456381     0.845667019    -0.000000066
   1.000000000    -0.424274534     0.441053468     0.500000000     0.500000000    -0.000000000     0.029473266    -5.711271785
   0.029473266     1.882106935     0.844028263    -0.000000068
   1.000000000    -0.424079395     0.440967081     0.500000000     0.500000000     0.000000000     0.029516459    -5.703120288
   0.029516459     1.881934163     0.843045662    -0.000000069
   1.000000000    -0.423955505     0.440905505     0.500000000     0.500000000    -0.000000000     0.029547247    -5.701530335
   0.029547247     1.881811010     0.842643217    -0.000000069
   1.000000000    -0.423902823     0.440881897     0.500000000     0.500000000     0.000000000     0.029559051    -5.700595511
   0.029559051     1.881763794     0.842387332    -0.000000069
   1.000000000    -0.423877210     0.440871437     0.500000000     0.500000000     0.000000000     0.029564282    -5.700289121
   0.029564282     1.881742873     0.842247855    -0.000000069
   1.000000000    -0.423878366     0.440874708     0.500000000     0.500000000    -0.000000000     0.029562646    -5.699609901
   0.029562646     1.881749415     0.842169190    -0.000000069
   1.000000000    -0.423868434     0.440871112     0.500000000     0.500000000     0.000000000     0.029564444    -5.699478928
   0.029564444     1.881742224     0.842103932    -0.000000069
```

ex: local greens function

```
[giacomo@work-laptop 16:06 uloc-2.00 (master)]$
[giacomo@work-laptop 16:06 uloc-2.00 (master)]$ more Gloc_l11_s1_iw.dat
   3.1415926535897933E-003  -5.8464619279676357E-003   3.5516409962760981E-014
   9.4247779607693795E-003  -1.7535285504820551E-002   3.5539022354320882E-014
   1.5707963267948967E-002  -2.9211819302948156E-002   3.5234510621651172E-014
   2.1991148575128554E-002  -4.0867906932570239E-002   3.4722712986129389E-014
   2.8274333882308138E-002  -5.2495446968694640E-002   3.5384753937703350E-014
   3.4557519189487726E-002  -6.4086414480951412E-002   3.5313122055419949E-014
   4.0840704496667310E-002  -7.5632882113037023E-002   3.5617349185019381E-014
   4.7123889803846901E-002  -8.7127040591108998E-002   3.5608851750492526E-014
   5.3407075111026485E-002  -9.8561218546315860E-002   3.5544253629803124E-014
   5.9690260418206076E-002 -0.10992790154358732        3.6191108974698710E-014
   6.5973445725385660E-002 -0.12121975021676776        3.6046998177184653E-014
   7.2256631032565244E-002 -0.13242961741897513        3.6949074713483326E-014
   7.8539816339744828E-002 -0.14355056430665492        3.7058253872252617E-014
   8.4823001646924426E-002 -0.15457587528593181        3.7812655296395187E-014
```

$$\omega_n = \frac{\pi}{\beta}(2n+1) \qquad \mathrm{Im}G(i\omega_n) \qquad \mathrm{Re}G(i\omega_n)$$

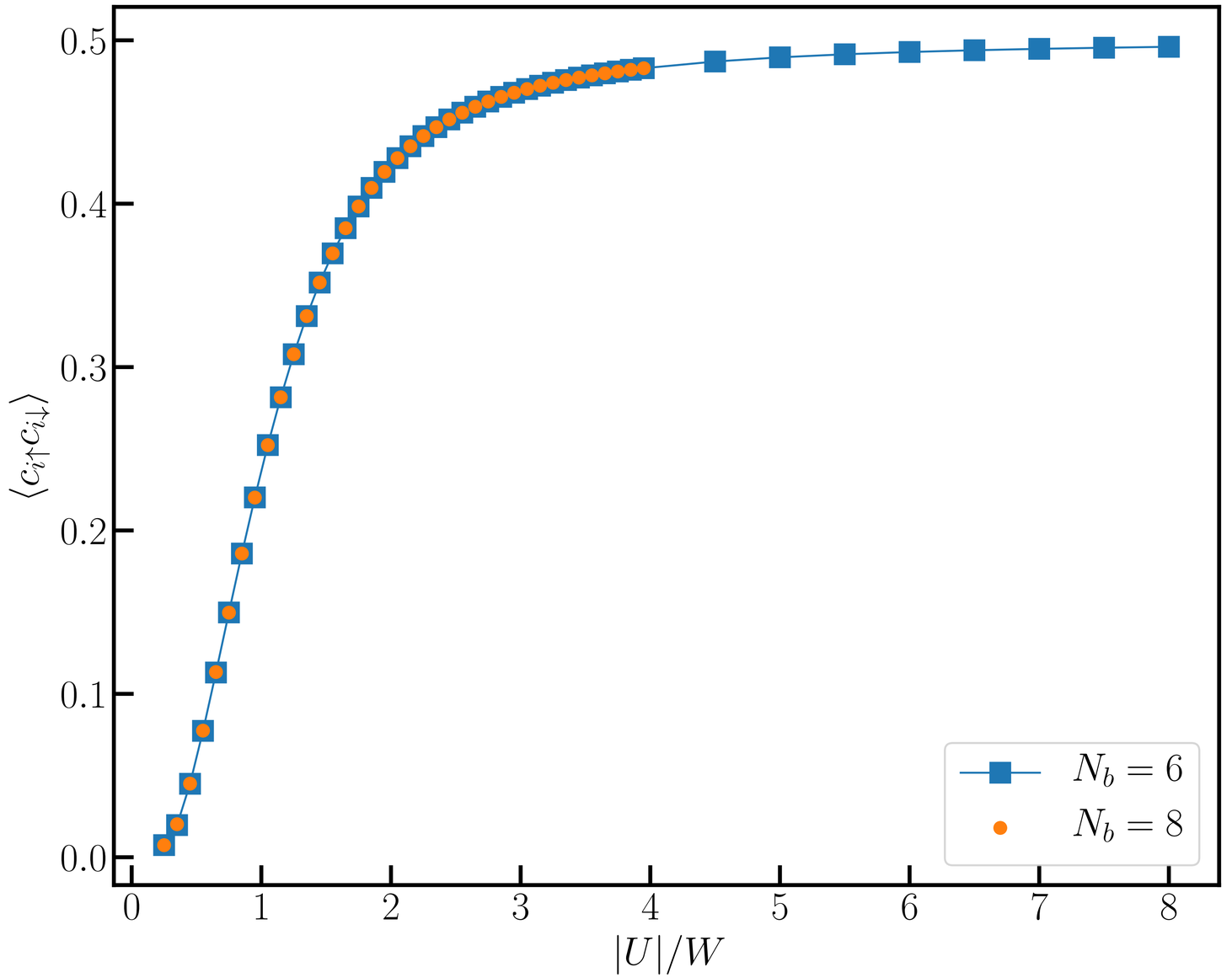
ex.: local energy $\langle H_i \rangle$

```
[giacomo@work-laptop 16:12 uloc-2.00 (master)]$ cat energy_info.ed energy_last.ed
#          1<Hi>  2<V>=<Hi-Ehf>        3<Eloc>         4<Ehf>         5<Dst>         6<Dnd>         7<Dse>         8<Dph>
   -0.381742224   -0.881742224    0.000000000    0.500000000    0.000000000    0.000000000    0.000000000    0.000000000
```

ex.: kinetic energy $K = -t \sum_{ij} \langle c^\dagger_{i\sigma} c_{j\sigma} \rangle$

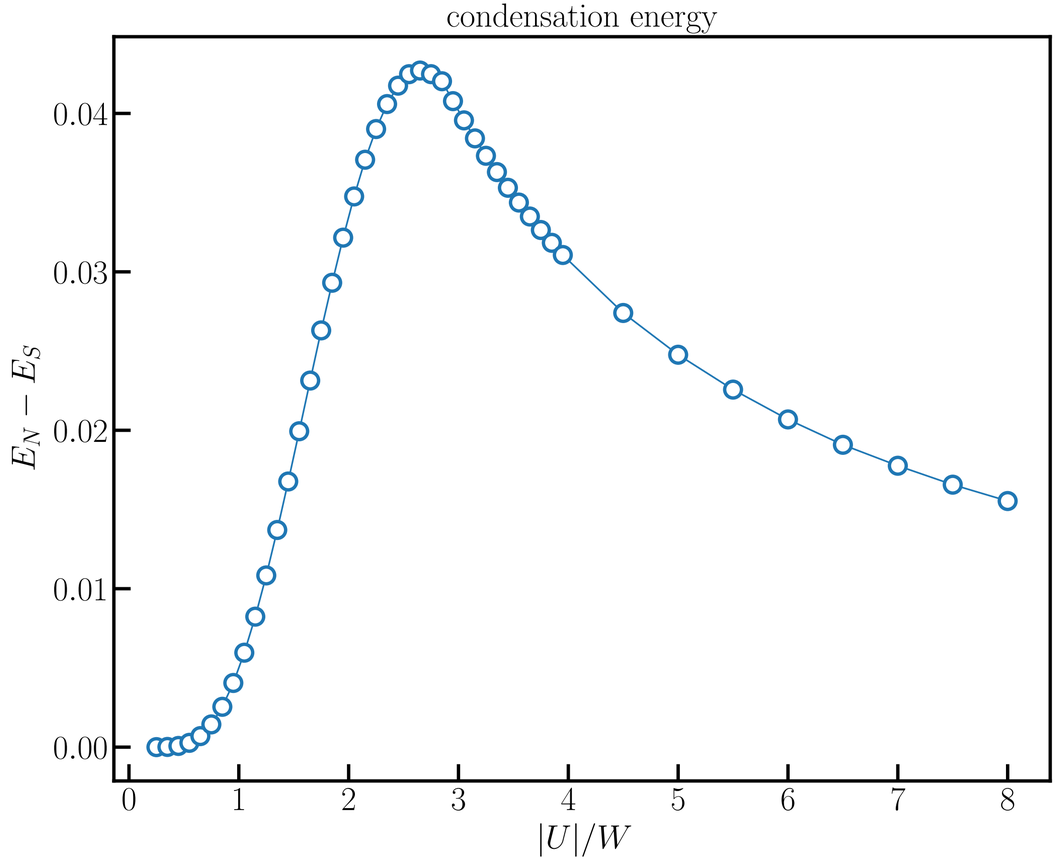
```
[giacomo@work-laptop 16:22 uloc-2.00 (master)]$ cat dmft_kinetic_energy.info dmft_kinetic_energy.dat
#           1<K>         2<Eloc>           3<K1>       4<Eloc1>
   -0.240864613    0.000000000   -0.240864613    0.000000000
```

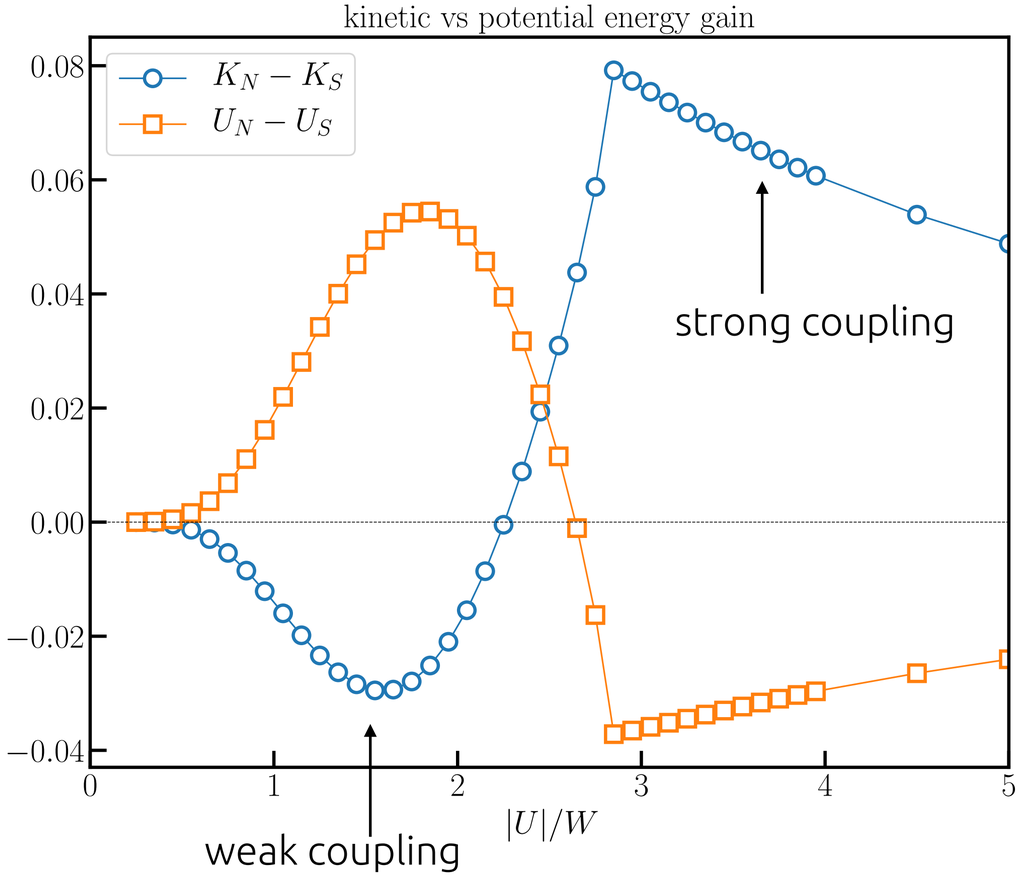
remember!!! total energy = kinetic energy + local energy


0.5
0.4
0.3
0.2
0.1
0.0
$\langle c_{i\uparrow} c_{i\downarrow} \rangle$
0
1
2
3
4
5
6
7
8
$|U|/W$
$N_b = 6$
$N_b = 8$

Make a run with ED_mode=superc and a run with ED_mode=normal to compute the condensation energy

follow the solution at different U and describe the weak to strong coupling crossover





for the braves: try a finite temperature calculation