U.S. DEPARTMENT OF ENERGY | Office of Science

COMSCOPE
from codes to spectroscopies

ComRISB--tutorials

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THE Ames Laboratory
Creating Materials & Energy Solutions
U.S. DEPARTMENT OF ENERGY

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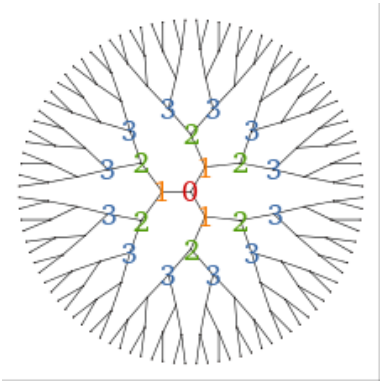
Examples

- Single-band Bethe lattice
- Single-band Checkboard lattice
- MnO
  a) Self-consistent calculation
  b) Special Mott-phase calculation
  c) Band structure analysis
- Ce

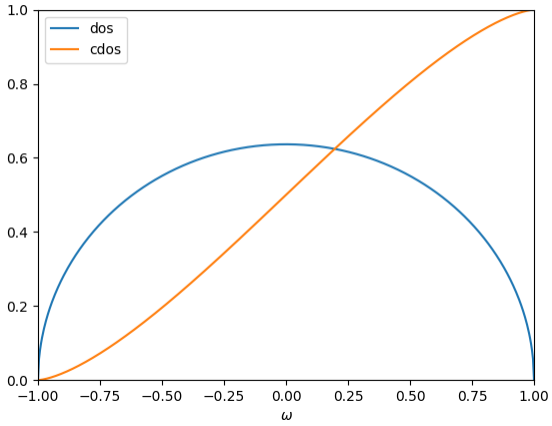
Single-band Bethe lattice

Objectives:

- Set up a simple model calculation
- Correlation induces metal-insulator transition in the G-RISB theory
- Measure the energy gap for the Mott-insulating phase



Bethe lattice with z=3



Bethe lattice with $z \to \infty$

Ref: https://cygutz.readthedocs.io/en/latest/tutorial_bethe_latt.html

Single-band Bethe lattice

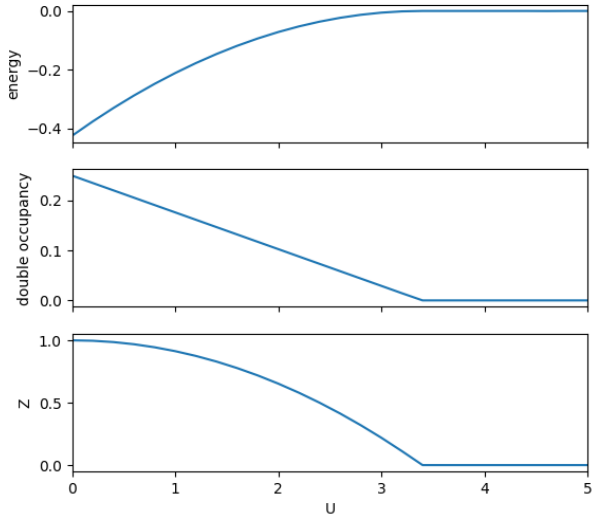
Scripts:

- Model: special.py (bare dispersion)
  semicir.py (G-RISB set up)
  scan_semicirc.py (main driver)

- Correlation-induced Mott transition:
  python ./scan_semicirc.py

- Question: what is the signature of Mott transition within G-RISB ansatz?

- Optional:
  1) submit job at scan_mu/scan_u.pbs
  2) python ./scan_semicirc.py



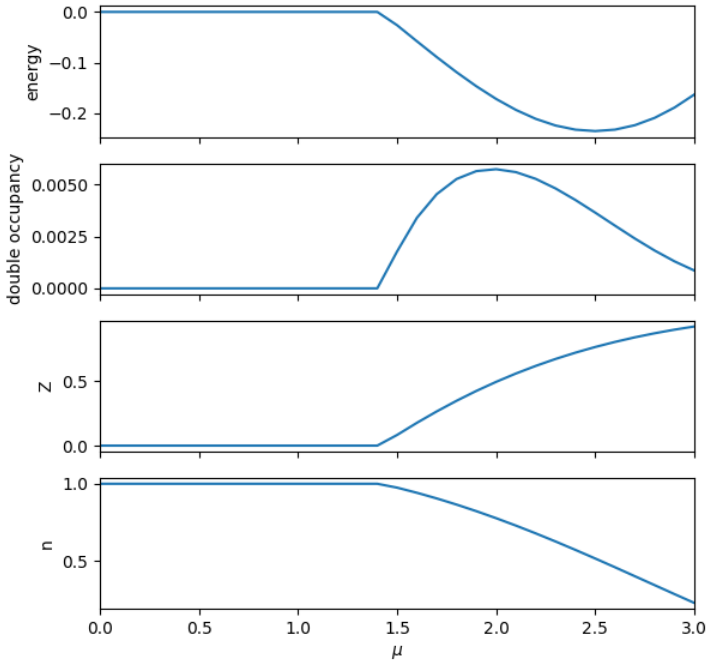
Single-band Bethe lattice

Scripts:

- Model: special.py (bare dispersion)
  semicir.py (G-RISB set up)
  scan_semicirc.py (main driver)

- Question: how to measure the band gap of Mott phase within G-RISB ansatz?
  python ./scan_semicirc.py -mu

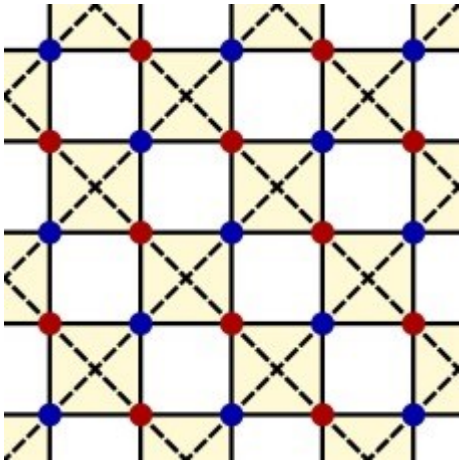
- Optional:
  1) submit job at scan_mu/scan_mu.pbs
  2) python ./scan_semicirc.py -mu



Single-band checkboard lattice

Objectives:

- How to set up a finite dimension (e.g., 2D) lattice with multiple sites per unit cell.
- How to setup simple antiferromagnetic (AFM) calculations.
- How the Gutzwiller method improves the descriptions at Hartree-Fock mean field level.

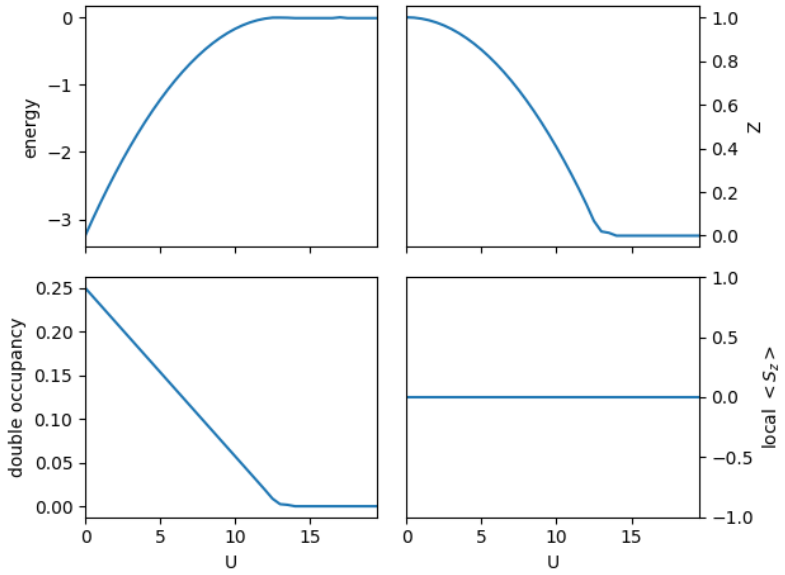


Ref: https://cygutz.readthedocs.io/en/latest/tutorial_checkboard.html

Single-band checkboard lattice

Scripts:

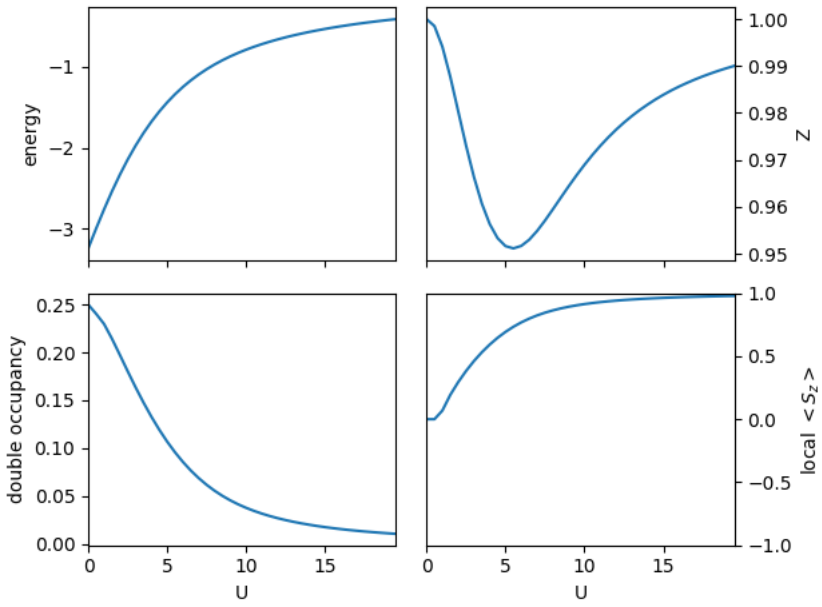
- Model: checkboard.py
  scan_checkboard.py (main driver)
- Mott transition:
  python ./scan_checkboard.py
- Question: critical U for Mott transition?
  Order of Mott transition?



Single-band checkboard lattice

Scripts:

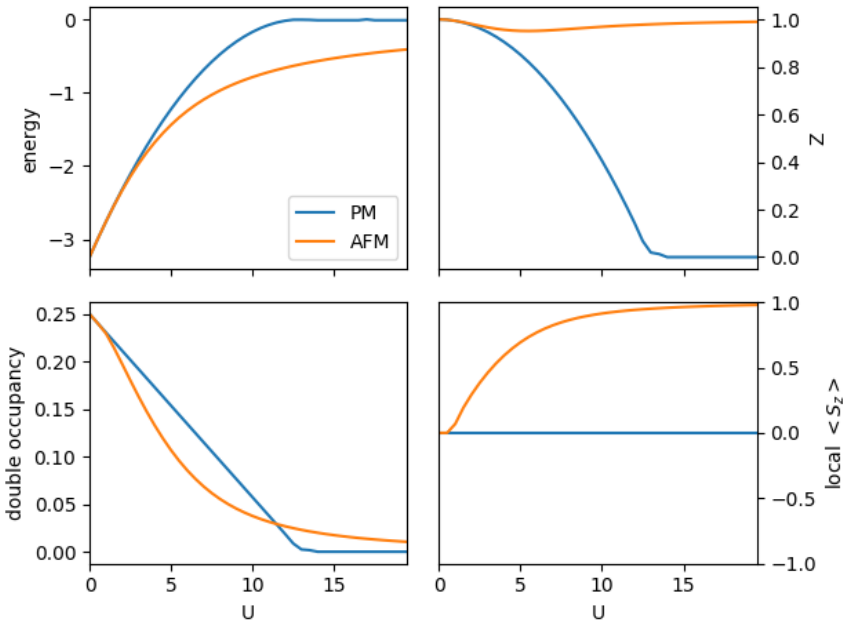
- Model: checkboard.py
  scan_checkboard.py (main driver)
- AFM phase:
  python ./scan_checkboard.py -sp



Single-band checkboard lattice

Scripts:

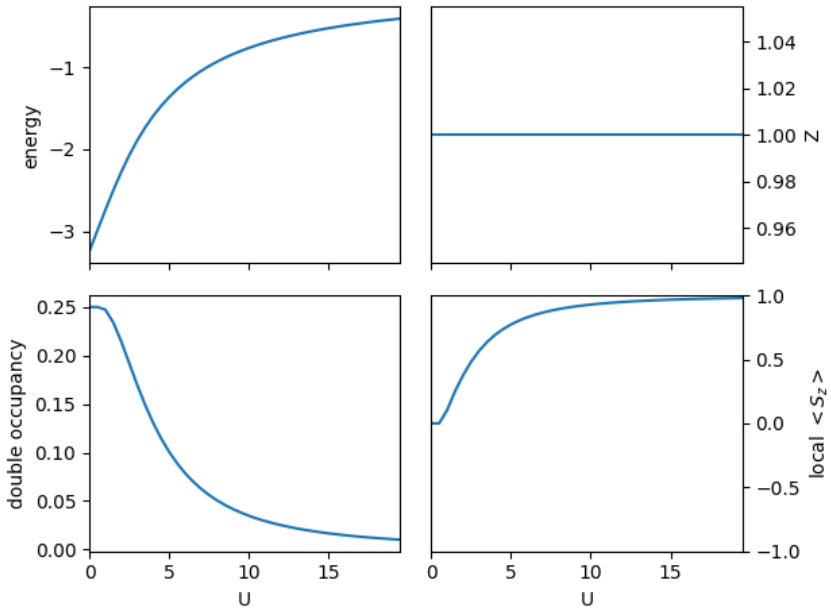
- Model: checkboard.py
  scan_checkboard.py (main driver)
- PM vs AFM phase:
  python ./plot_pmafm.py



Single-band checkboard lattice

Scripts:

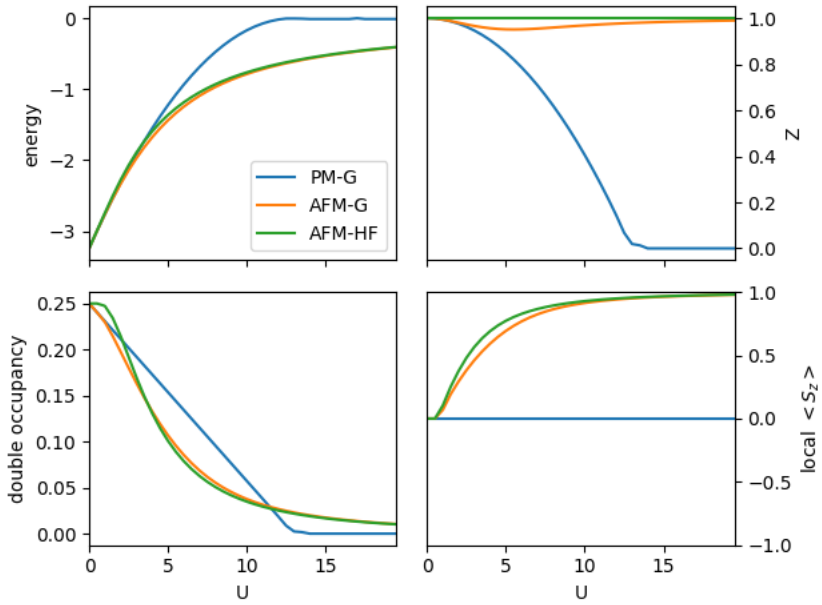
- Model: checkboard.py
  scan_checkboard.py (main driver)
- PM vs AFM phase:
  python ./scan_checkboard.py -uhf



Single-band checkboard lattice

Scripts:

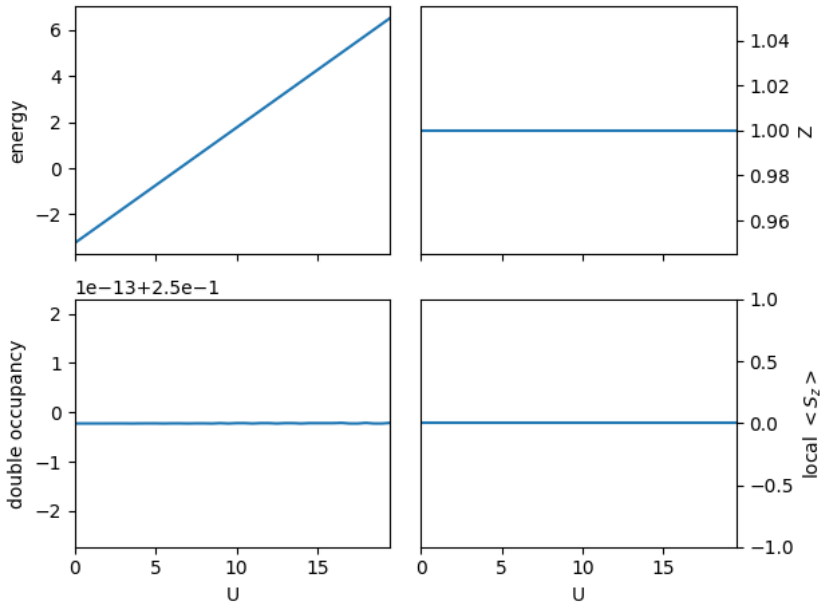
- Model: checkboard.py
  scan_checkboard.py (main driver)
- PM vs AFM solutions:
  python ./plot_pmafm_gh.py



Single-band checkboard lattice

Scripts:

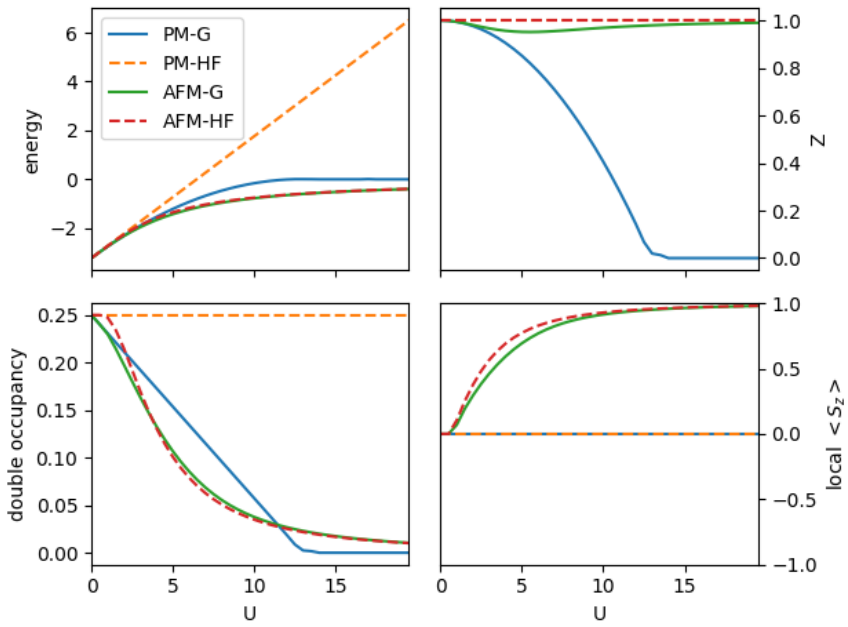
- Model: checkboard.py
  scan_checkboard.py (main driver)
- HF calculation:
  python ./scan_checkboard.py -rhf



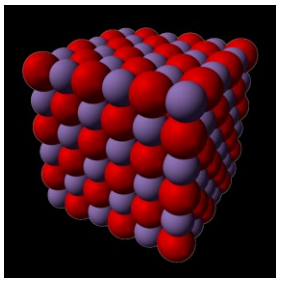
Single-band checkboard lattice

Scripts:

- Model: checkboard.py
  scan_checkboard.py (main driver)
- Overall comparisons:
  python ./plot_pmafm_gh2.py



MnO



Background data:

Rock salt structure

$T_N \approx 116K; gap \approx 2.6eV$

Objective:

(a) basic steps to run DFT+G-RISB calculations

(b) Monitoring job (if desired)

(c) key input/output files

(d) Basic band structure analysis

(e) Handle multiple solutions—special Mott solver

MnO

DFT (LDA) input file: **ini**

Note: $10 \times 10 \times 10$ k-mesh

Calculation results in directory **tutorials/MnO/dft/**

DFT+G-RISB input file: **comdmft.ini**

```
control={'initial_lattice_dir' : '../dft/',
'method' : 'lda+risb', # either lda+dmft or lqsgw+dmft,
'spin_orbit' : False, # True or False. spin-orbit coupling is included or not
'mpi_prefix': "mpirun -np 8",
'impurity_problem':[[1, 'd']],
'impurity_problem_equivalence':[1],
'max_iter_num_outer': 2
}
imp={'temperature' : 300, # temperature (in K)
'1':
{
'f0': 9.0,
'f2': 9.82,
'f4': 6.13,
'nominal_n': 5.0,
```

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Job submission script:

comrisb_mno.pbs

```
#PBS -N MnO
#PBS -S /bin/bash
#PBS -l nodes=n029:ppn=8
#PBS -l walltime=5:55:5

module purge
module load gcc
module load intel/PSXE2018.u2
module load comsuite/V1-2018.intel-PSXE2018-u2.openmpi-2.0.1
# module load comsuite/V1-2018.intel-PSXE2018-u2.openmpi-2.0.1_RISB
source activate py27

export SOURCE="$PBS_O_WORKDIR"
export WORKDIR="$PBS_O_WORKDIR"

cd $WORKDIR

echo "--] Running job on " `hostname`
echo Begin: `date`
echo

# mkdir -p dft
# cd dft
# cp ../ini .
# mpirun -np 8 rspflapw.exe
# cd ..
mkdir -p dft_risb
cd dft_risb
cp ../comdmft.ini .
comrisb.py

echo
echo End: `date`
```

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Job monitoring:

cmd.log: sequential execution of modular binary files

top_dir /home/yxphysics/comrisb_tutorial/tutorials/MnO/dft_risb
lattice_directory
/home/yxphysics/comrisb_tutorial/tutorials/MnO/dft_risb/lattice
wannier_directory
/home/yxphysics/comrisb_tutorial/tutorials/MnO/dft_risb/wannier
lowh_directory
/home/yxphysics/comrisb_tutorial/tutorials/MnO/dft_risb/lowh

****

iteration: 1
****

initial dft directory setup done.
mpirun -np 8 /opt/WinterSchool2019/COMSUITE/bin/**ComWann**
comwann start at 17/02/2019 10:13:14 end at 17/02/2019 10:14:49
reading wannier.inip to get basis information.
control['impurity_wan']: [[4, 5, 6, 7, 8]]
mpirun -np 8 /opt/WinterSchool2019/COMSUITE/bin/**gwannier.py**
gwannier start at 17/02/2019 10:14:49 end at 17/02/2019 10:15:28
mpirun -np 8 /opt/WinterSchool2019/COMSUITE/bin/**CyGutz** -r 0
cygutz start at 17/02/2019 10:15:34 end at 17/02/2019 10:21:37
mpirun -np 8 /opt/WinterSchool2019/COMSUITE/bin/**gwannden.py**
gwannden start at 17/02/2019 10:21:38 end at 17/02/2019 10:21:47
prepare_dft_input done.
dft calculation done.

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Job monitoring:

convergence.log

i_outer	delta_rho	etot	mu	err_risb	min_z
1	0.00512815	-2462.45607932	1.42564821	0.00000023	0.50765420
2	0.00195214	-2462.46559867	1.42558328	0.00000095	0.50767527
3	0.00052596	-2462.47117647	1.53955005	0.00000068	0.49626877
4	0.00021339	-2462.47321781	1.61397272	0.00000007	0.48503757
5	0.00013063	-2462.47410896	1.64020025	0.00000025	0.48572462
…….					
25	0.00000055	-2462.47626490	1.66672910	0.00000018	0.48727939
26	0.00000043	-2462.47627620	1.66688257	0.00000040	0.48726555
27	0.00000033	-2462.47628607	1.66702294	0.00000007	0.48725332
28	0.00000026	-2462.47629459	1.66714464	0.00000007	0.48724234

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Output file: **lowh/GUTZ.LOG**

Bare orbital levels/splittings

```
************      h1e-sym  ************
 imp=  1
 real part
  -0.4466   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000  -0.4466   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000  -0.4466   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000  -0.4466   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000  -0.4466   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000  -0.4466   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000  -0.2899   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000  -0.2899   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000  -0.2899   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000  -0.2899
 orbital splitting:
   0.00000   0.00000   0.00000   0.00000   0.00000   0.00000   0.15672   0.15672   0.15672
0.15672
```

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Output file: **lowh/GUTZ.LOG**

Bare orbital occupancies $\langle \Psi_0 | d^\dagger_{\alpha\sigma} d_{\beta\sigma} | \Psi_0 \rangle$

```
************      nks-sym  ************
 imp=  1
 real part
   0.6887   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.6887   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.6887   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.6887   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.6887   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.6887   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.3695   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.3695   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.3695   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.3695
 sub_tot=  5.610245 -0.000000
```

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Output file: **lowh/GUTZ.LOG**

Renormalized quasiparticle orbital occupancies $\langle \Psi_0^{opt.} | d_{\alpha\sigma}^{\dagger} d_{\beta\sigma} | \Psi_0^{opt.} \rangle$

```
************      nks-sym  ************
 imp=  1
 real part
   0.8118   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.8118   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.8118   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.8118   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.8118   0.0000   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.8118   0.0000   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0765   0.0000   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0765   0.0000   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0765   0.0000
   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0765
 sub_tot=  5.176857  0.000000
```

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Output file: **lowh/GUTZ.LOG**

Renormalization matrix

$$Z = R^{\dagger} R$$

********** z-out-sym **********

imp= 1

real part

0.4872	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.4872	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.4872	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.4872	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.4872	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.4872	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8071	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8071	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8071	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.8071

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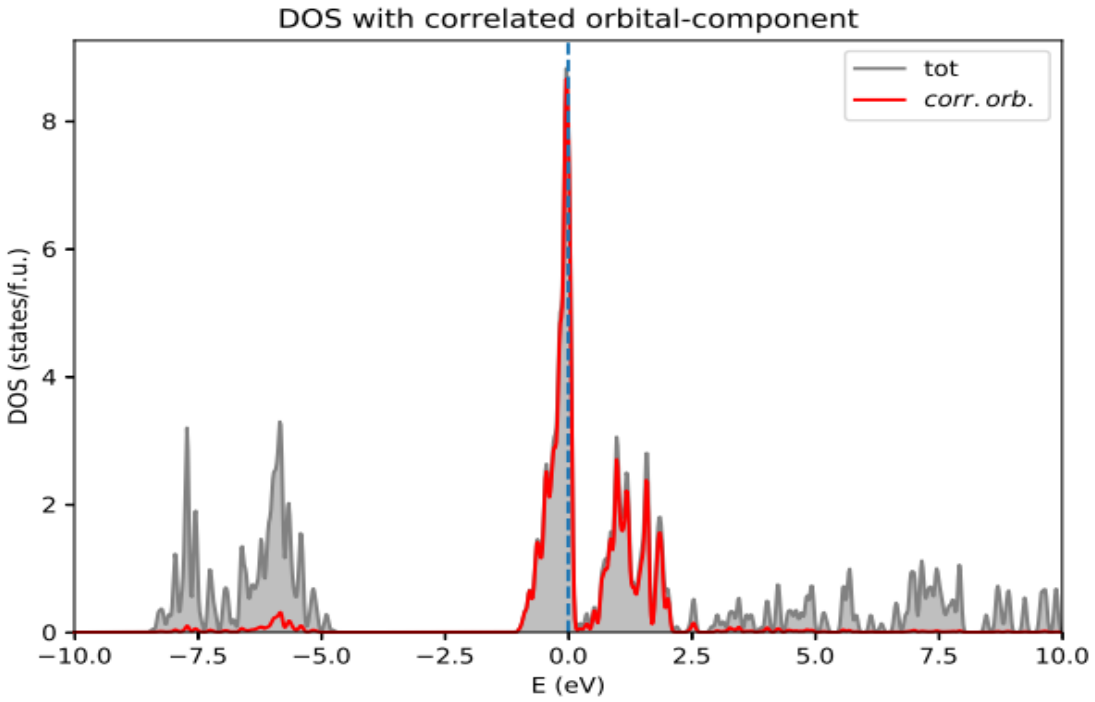
Quasi-particle DOS:

${COMSUITE_BIN}/plot_dos_tf.py -el -10 -eh 10



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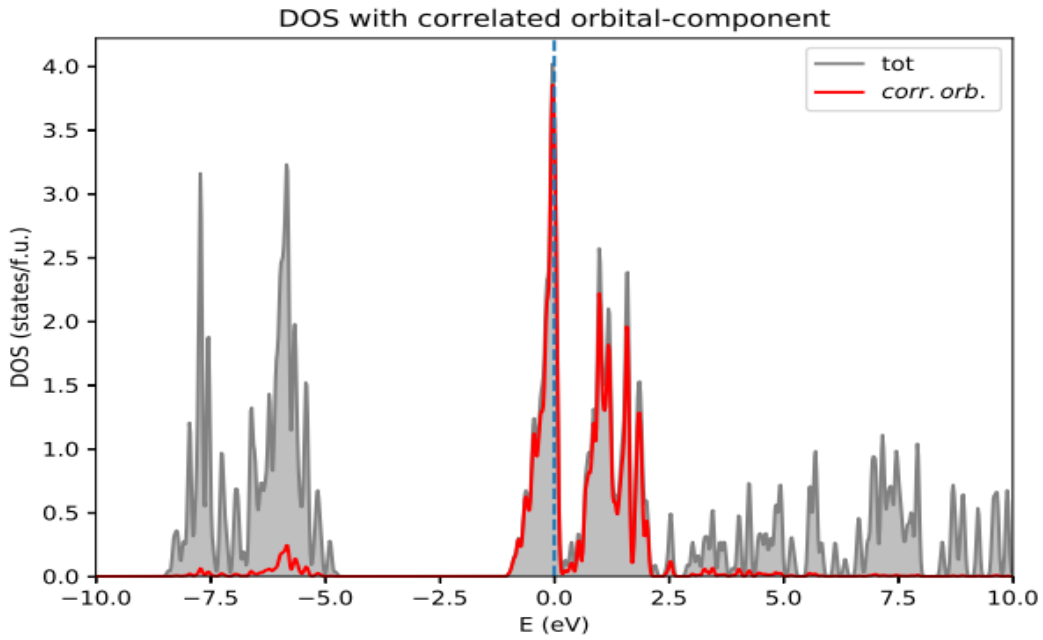
Coherent part of DOS:

${COMSUITE_BIN}/plot_dos_tf.py -el -10 -eh 10 -ch



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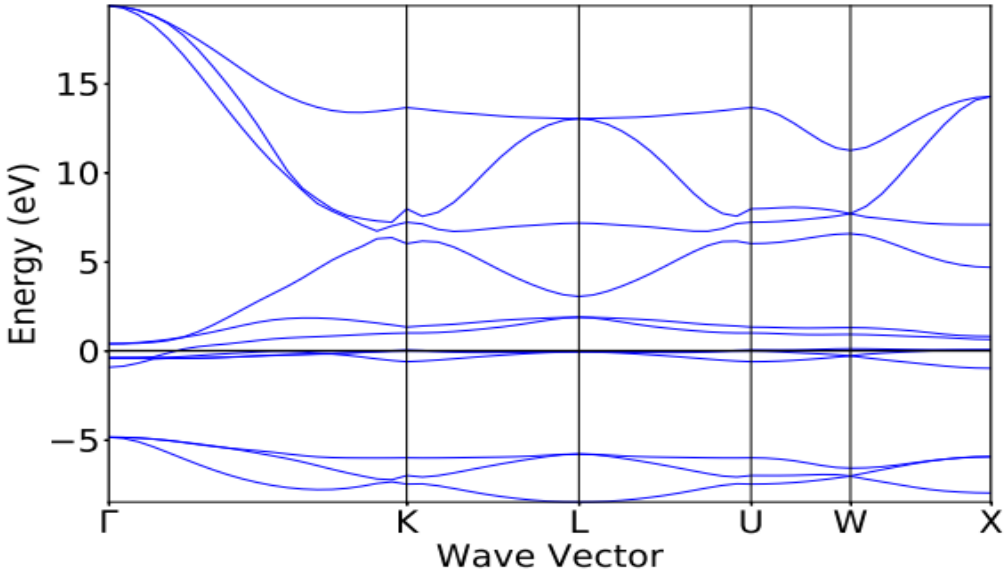
Quasiparticle band structure:

mpirun -np 4 ${COMSUITE_BIN}/gwannier_plot_bands.py -g



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Multiple solutions and special Mott solvers:

Create another folder:

cp –r lowh lowh_mott

Set up Mott calculations:

${COMSUITE_BIN}/init_mott.py

```
********** Impurity 1 **********
 Sigma structure:
index    0   1   2   3   4   5   6   7   8   9

  0     1   0   0   0   0   0   0   0   0   0
  1     0   1   0   0   0   0   0   0   0   0
  2     0   0   1   0   0   0   0   0   0   0
  3     0   0   0   1   0   0   0   0   0   0
  4     0   0   0   0   1   0   0   0   0   0
  5     0   0   0   0   0   1   0   0   0   0
  6     0   0   0   0   0   0   2   0   0   0
  7     0   0   0   0   0   0   0   2   0   0
  8     0   0   0   0   0   0   0   0   2   0
  9     0   0   0   0   0   0   0   0   0   2
 Please provide the indices of orbitals to be Mott localized
 (e.g., 0 2 ): 0   1   2   3   4   5   6   7   8   9
 You selected [0   1   2   3   4   5   6   7   8   9]
 to be Mott localized, right? (y/n):y
 Please provide the total number of Mott localized electrons (per
unit cell): 5
 Total 5 electrons will be Mott localized, right? (y/n):y
Please select the method to solve embedding Hamiltonian.
 LDIAG = -2: Valence truncation ED for Mott solution.
        -3: Option (-2) with additional S=0 constraints.
        -4: Option (-2) with additional J=0 constraints.
       -31: Option (-2) with S=0
            and local symmetry constraints.
 Please select LDIAG:
 Pick one from [-2, -3, -4, -31]...-3
```

MnO

Run G-RISB calculation:

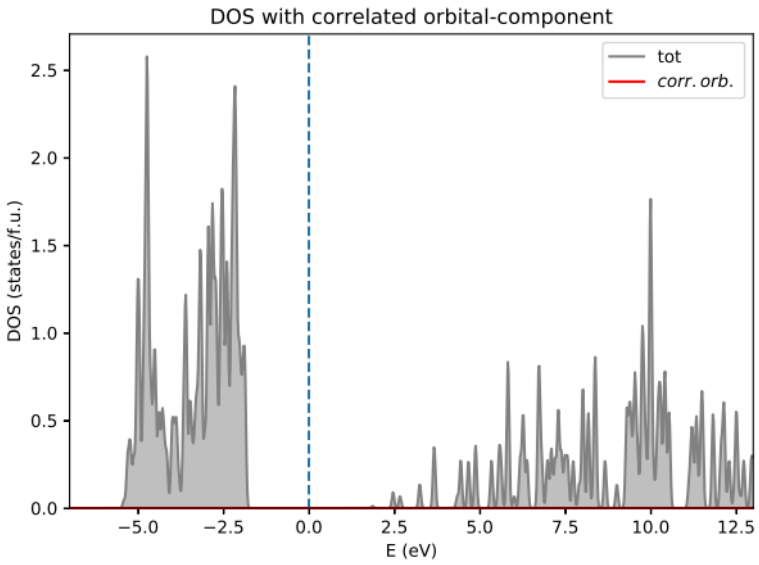
mpirun -np 8 CyGutz -r 0

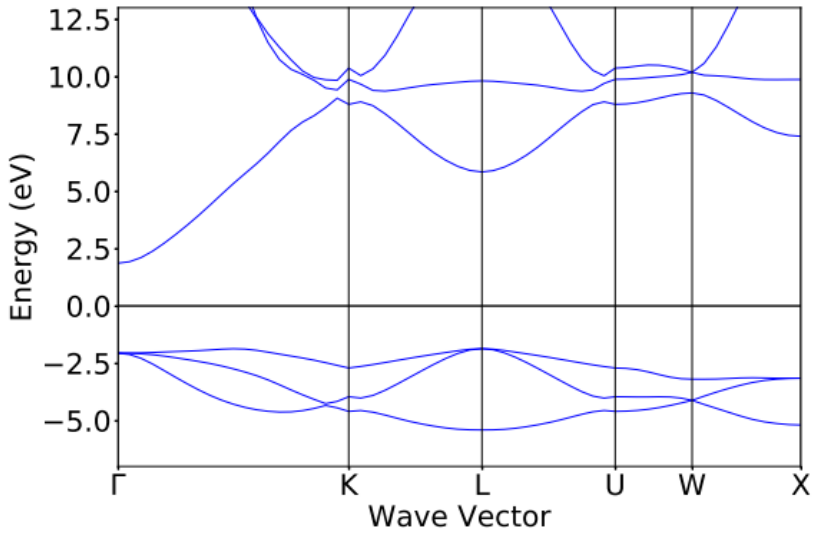
Plot band structure (coherent part):

mpirun -np 4 ${COMSUITE_BIN}/gwannier_plot_bands.py –g

Plot DOS (coherent part)

${COMSUITE_BIN}/plot_dos_tf.py -el -10 -eh 10 -ch





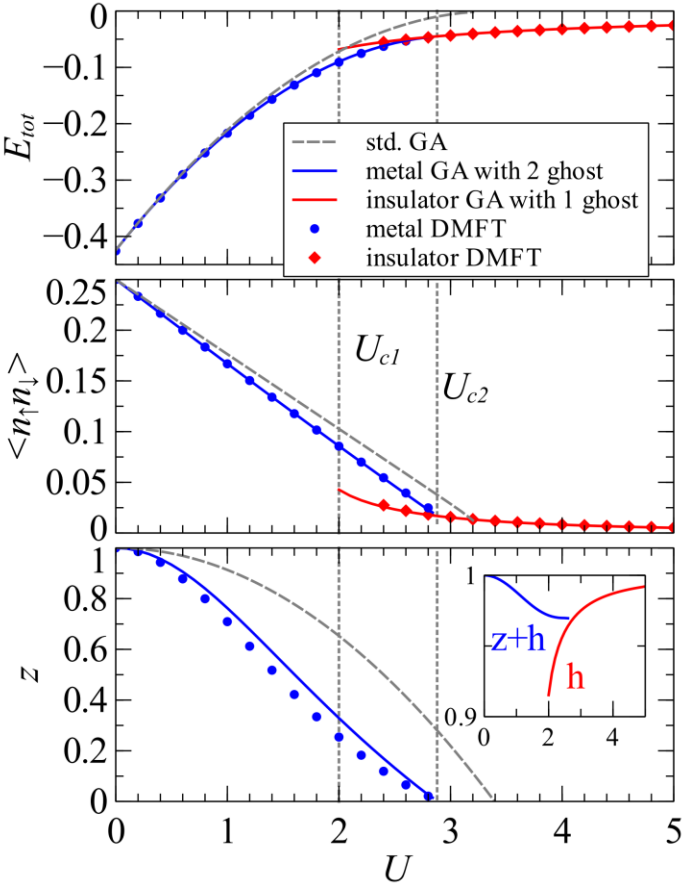
Ce

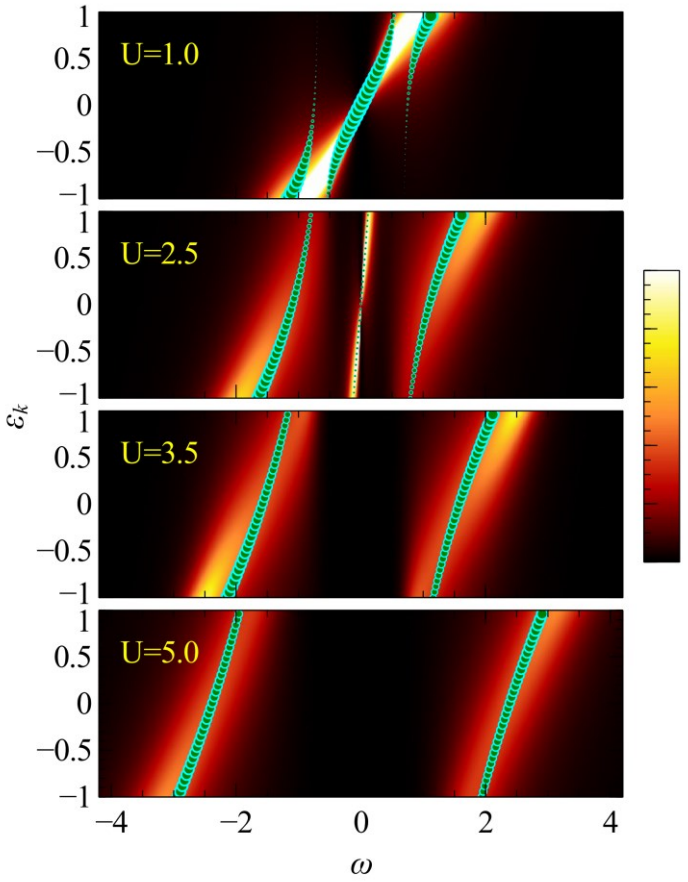
Repeat the calculations and analysis for Ce.

Ref: https://cygutz.readthedocs.io/en/latest/tutorial_alpha_ce.html

Thank You!

Appendix: Bethe lattice





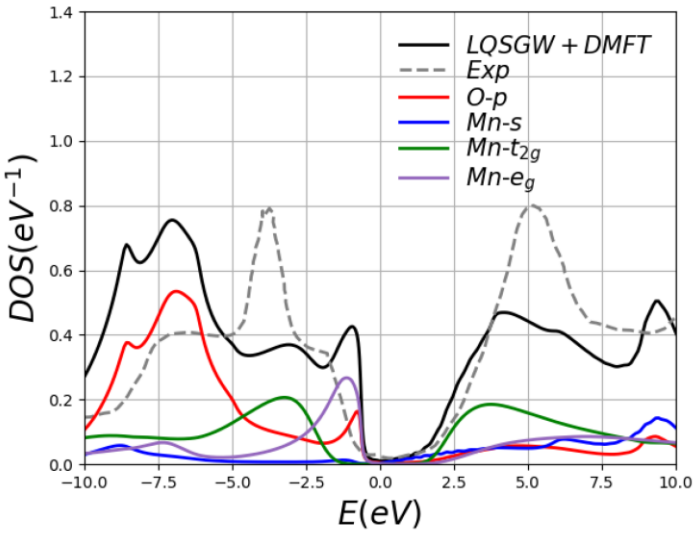
Lanatà, Nicola, Tsung-Han Lee, Yong-Xin Yao, and Vladimir Dobrosavljević. 2017. “Emergent Bloch Excitations in Mott Matter.” *Physical Review B* 96 (19): 195126.

substance: MnO
property: band structure, energy gap

Brillouin zone: Fig. 1, partial APW band structure: Fig. 2. This calculation overestimates the O 2p – Mn 3d energy separation [78K].

energy gaps

$E_{g,th}$	2.43(8) eV		from transport data	67H
	2.6 eV			68A
	2.6(2) eV			71G
	$1.90–6\cdot10^{-4}T$ eV		T in K	76K
	2.7...3.0 eV		from photoconductivity, Fig. 3	77U
E_g	3.6 eV	$T = 300$ K	from UV absorption; shift of 500 cm^{-1} in E_g below T_N	74C



MnO DOS within LQSGW+DMFT. For comparison, experimental data is marked by a gray dashed line. LQSGW+DMFT reproduces the experimentally observed four peak structure at 5eV, -2eV, -4eV and -7eV relative to the Fermi energy reasonably well. A projected density of state calculation attributes each peak to Mn-t_{2g}, Mn-e_g, Mn-t_{2g}, and O-p orbitals, respectively. A substantial contribution of O-p to the top of the valence band is a manifestation of strong hybridization between O-p and Mn-e_g, which is consistent with the Zhang-Rice picture.