User-guide for MO-IPT package.

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1 Brief description

MO-IPT stands for multi-orbital iterated perturbation theory. The present code implements the MO-IPT solver as described in Dasari et al [paper reference] within the dynamical mean field theory (DMFT) framework and may be used to obtain single- -particle spectra and self-energies for strongly correlated model Hamiltonians as well as real materials with multiple orbital degrees of freedom. The code is implemented for zero as well as finite temperatures. The impurity solver uses the second-order self-energy in an ansatz motivated by the continued fraction expansion of the self- -energy. The ansatz has certain free parameters that are chosen to satisfy high frequency and the atomic limits. Since the ansatz reproduces low frequency Fermi liquid behaviour and the band limit by construction, the MO-IPT is expected to be a reasonable interpolating approximation. Naturally, the MO-IPT cannot be expected to be accurate close to phase transitions, etc, where exact methods such as QMC and NRG would be far more accurate. For extensive benchmarking of the method with continuous time Monte Carlo and other methods, please see Dasari et al [paper reference]. The main limitation of the code is that the Hund's coupling is presently considered only as a density-density interaction. The main merits of the MO-IPT is that it is fast, numerically inexpensive, can deal with many orbitals, and provides real frequency results at zero and finite temperature. The main motivation of our implementation is to carry out first principles calculations of strongly correlated materials, so the integration with band structure results (from e.g WIEN2K) is also implemented in this set of codes.

2 Quick build and execution

- cd MO-IPT/src; make clean
- make
- cd ..; chmod 755 run.sh; ./run.sh

This is an interactive script. There are five sample data sets. For the 1st and 2nd data sets, the number of recommended MPI processes, np, is one, while for the rest, some speedup is achieved by $np > 1$.

3 Directory Structure

The package has the following directory structure:

README

COPYRIGHT.txt

docs/ Documentation

- manual.pdf // Detailed instructions and guide
- flowchart.pdf // Flowchart for MO-IPT

data/ Example calculations. Each sample set has an `input/` and an `output/` subdirectory.

- sample_1/ and sample_2/ // Examples for model Hamiltonian calculations with toy density of states
- sample_3/ and sample_4/ // Examples for real material calculations
- sample_5/ // Example for a model Hamiltonian calculation on a 2-D square lattice

src/ Source files

- Makefile
- main.f90 // Main program for MO-IPT calculation, DMFT iterations, self-energy calculation etc.
- makegrid.f90 // Module for creating real frequency (energy) grids.
- ksum.f90 // Module for momentum summation and constructing local Green's functions.
- funct.f // Collection of auxiliary modules like Fermi function, Hilbert transform, interpolation, root finder etc.
- Glob_cons // Global constants.

4 Input/Output description

The input files are described below:

- par.dat This is the most important input file for MO-IPT calculations. The structure of this file is giv

  b_1 ϵ_1 ϵ_2 b_2 db_2 ϵ_3 Grid parameters

  b_3 db_3 ϵ_4 ϵ_5 Grid parameters

  U J_H $dfac$ $correc$ $correc2$ t α $Jflag$

$phsym \;\; LDA\_DMFT \;\; init \;\; idos \;\; uniform\_grid$

$temp \;\; frac \;\; eta$

$Norbs \;\; Nkp \;\; NQPTS \;\; Ndim$

4.1 Input parameter description

The first two lines define an inhomogeneous frequency or energy grid, and are used in makegrid.f90.

U**:** represents local Coloumb repulsion (Hubbard - U).

J_H**:** stands for Ising type Hund's coupling.

$dfac$**:** This is mixing parameter between old and new solutions, and is used for smoother convergence.

$correc$**,** $correc2$ **:** These parameters are mixing fractions for two particle correlation (2PC) and three particle correlation (3PC) functions. So if $correc = 0.3$, then only 0.3 of the 2PC function enters the calculations. It is advised to keep $correc$ small for initial calculations and increase them gradually using converged data for lower $correc$ parameters.

t**:** Bare hopping integral for model calculations and in general is the unit of energy.

$Jflag$**:** This flag decides the format of $U - J$ matrix.

$phsym$**:** This flag can be used to enforce particle-hole symmetry. If $phsym = 0$, then the chemical potential is tuned to get the fixed total occupancy, else if $phsym = 1$, the occupancy of each orbital is fixed at 0.5 and the μ is set to zero.

LDA_DMFT**:** If $idos > 3$, then two options are available using the LDA_DMFT flag. If this flag is set to 1, then DMFT calculations will be carried out for a DFT-calculated $H_0(k)$. So an input file names HK_data will be expected. The number of Q-points used for the DFT calculation also need to be specified in the $NQPTS$ variable (see below). For other values of LDA_DMFT (and $idos \geq 4$), the model calculations with real density of states (2-D square or 3-D cubic) are carried out. The dimensionality $Ndim$ needs to be specified in this case.

$init$**:** init=0 means - start a fresh calculation and no previous data is available. init=1 means supply previously computed data as input.

$idos$**:** Flag for choice of non-interacting density of states.

idos=1 : Hypercubic lattice, Gaussian Density of states.

idos=2 : Bethe lattice or Cayley tree, semicircular density of states.

idos=3 : General (user supplied) density of states.

idos=4 : Real material calculations using LDA Tight - Binding input OR model calculations on a 2D square/3D cubic lattice.

uniform_grid: If this flag is set to 1, then a homogeneous ω-grid is created, else a logarithmic+homogeneous grid is generated.

temp: Temperature in units of t for model calculations or in eV when doing real-material calculations.

frac: Set default value as 0.

eta: Defines appropriate contour in the complex plane. It should be positive and typical value is of the order of 10^{-4}.

Norbs: is the total number of orbitals (including spin degeneracy). If N is the number of orbitals you are interested, then *Norbs* will take value $2N$. The factor 2 is because each orbital is considered to have two spin indices ($\uparrow$ or $\downarrow$).

Nkp: is the total number of k-points from 0 to π, and is made use of to generate a k-point mesh for real lattice calculations (with idos=4, LDA_DMFT=0, Ndim=2 or 3). The default value is 0.

NQPTS: The total number of K-points in the $H_0(k)$ produced by the DFT. For example, in the sample_3 and sample_4, the DFT was carried out using a $25 \times 25 \times$ K-point mesh, hence the $H_0(k)$ contains 15625 entries, and thus NQPTS=15625. This parameter is used only when doing real-material calculations (idos=4, LDA_DMFT=1). The default value is 0.

Ndim: The dimensionality of the lattice. This parameter is used in conjunction with *Nkp* when model calculations need to be performed on realistic 2D square or 3D cubic lattices. For these $Ndim = 2$ or 3 respectively must be specified. See also the description for LDA_DMFT above.

- initials.dat: This is another input file that contains initial occupancies and chemical potentials. The structure of the file is given below:
  $n_{1\uparrow}$
  $n_{1\downarrow}$
  $n_{2\uparrow}$
  $n_{2\downarrow}$
  .
  .
  .
  .
  .
  .
  .
  $n_{N\uparrow}$
  $n_{N\downarrow}$
  μ_{guess}, $\mu_{0\,guess}$, $FermiLevel(DFT)$
  ntotinput

occupancies : $n_{r\uparrow}$ is the occupancy of the r$^{\text{th}}$ orbital for up spin and $n_{r\downarrow}$ is the occupancy of the r$^{\text{th}}$ orbital for down spin.

μ_{guess} : User-provided guess value of μ so that total occupancy constraint is satisfied. The code finds appropriate μ given a fixed total occupancy, n_{tot}.

$\mu_{0\,guess}$: User-provided guess pseudo-chemical potential for satisfying Luttinger's Theorem (LT). The code does not modify this automatically, and at present a manual tuning of μ_0 is required to satisfy the LT.

$FermiLevel(DFT)$: For real material calculations, it is the Fermi energy calculated by DFT.

ntotinput Total occupancy of all the orbitals considered in the calculation. This is a fixed number for a given calculation.

- HK_data

  This input file represents a non-interacting Hamiltonian matrix in the orbitals basis for several momentum values. Mathematically, this is denoted as $H_0(\mathbf{k})$. This input is needed when $idos = 4$ and $LDA_DMFT = 1$. which is the combination appropriate for first principles based real material calculations and is derived from DFT calculations followed by downfolding. The structure of this input file is given below:

$$H_0(k) = \begin{pmatrix} P_n(k_1) \\ P_n(k_2) \\ \vdots \\ \vdots \\ P_n(k_{NQPTS}) \end{pmatrix} \tag{1}$$

where each of the $P_n(k)$ are one-dimensional column vectors given by

$$P_n(k) = \begin{pmatrix} H_{1\uparrow,1\uparrow}(k) \\ H_{1\uparrow,1\downarrow}(k) \\ H_{1\uparrow,2\uparrow}(k) \\ H_{1\uparrow,2\downarrow}(k) \\ \cdots \\ H_{1\uparrow,n\uparrow} \\ H_{1\uparrow,n\downarrow} \\ H_{1\downarrow,1\uparrow}(k) \\ H_{1\downarrow,1\downarrow}(k) \\ H_{1\downarrow,2\uparrow}(k) \\ H_{1\downarrow,2\downarrow}(k) \\ \cdots \\ H_{1\downarrow,n\uparrow} \\ H_{1\downarrow,n\downarrow} \\ \vdots \\ \vdots \\ H_{n\uparrow,1\uparrow}(k) \\ H_{n\uparrow,1\downarrow}(k) \\ H_{n\uparrow,2\uparrow}(k) \\ H_{n\uparrow,2\downarrow}(k) \\ \cdots \\ H_{n\uparrow,n\uparrow} \\ H_{n\uparrow,n\downarrow} \\ H_{n\downarrow,1\uparrow}(k) \\ H_{n\downarrow,1\downarrow}(k) \\ H_{n\downarrow,2\uparrow}(k) \\ H_{n\downarrow,2\downarrow}(k) \\ \cdots \\ H_{n\downarrow,n\uparrow} \\ H_{n\downarrow,n\downarrow} \end{pmatrix} \tag{2}$$

The following are the main output files:

- Green's functions

  The computed Green's functions are written in Gf1.dat for the 1$^{\text{st}}$ orbital, spin $\uparrow$, Gf2.dat for the 1$^{\text{st}}$ orbital, spin $\downarrow$, Gf3.dat for the 2$^{\text{nd}}$ orbital, spin $\uparrow$, and so on.

  In each file there are three columns. The first column is frequency, the second is the positive definite spectral function and the third column is the real part of the Green's function.

- Self energy

  The calculated self-energies are written in sig1up.dat file for the 1$^{\text{st}}$ orbital, up spin and sig1down.dat file for the 1$^{\text{st}}$ orbital, down spin. And similarly for the 2$^{\text{nd}}$ orbital, sig2up.dat and sig2down.dat files contain self-energies for up and down spins respectively. In each file, frequency is in the 1st

column, imaginary part of the self-energy is in the second column and real part of the self energy is in the third column.

- quasiwei.dat

  Calculated quasi-particle weights are written in this file.

- interaction matrix.dat

  The interaction matrix is written in this file.

- Mastubara_self.dat

  The self-energies computed on the real frequency axis are Fourier transformed to Matsubara frequencies and then written to this file. The first column is the $\omega_n = (2n+1)\pi T$, where T is the temperature, and the rest of the columns are imaginary parts of the up-spin self-energies of the orbitals, i.e $\mathrm{Im}(\Sigma_{1\uparrow}(i\omega_n))$, $\mathrm{Im}(\Sigma_{2\uparrow}(i\omega_n))$ and so on. Currently $n \in [-300 : 300]$.

- Mastubara_green.dat

  The Green's functions computed on the real frequency axis are Fourier transformed to Matsubara frequencies and then written to this file. The format is similar to the self-energy file above, except that the self-energy is replaced by the corresponding Green's function.

5 System information

The codes have been tested on the following system configurations:

- Ubuntu on Intel Xeon Hex-core E5645 (2.4GHz) with 12GB RAM
  - `uname -a`

    Linux 3.2.0-23-generic 36 -Ubuntu SMP Tue Apr 10 20:39:51 UTC 2012 x86_64 x86_64 x86_64 GNU/Linux
  - `lsb_release -a`

    DISTRIB ID=Ubuntu
    DISTRIB RELEASE = 12.04
    DISTRIB CODENAME=precise
    DISTRIB DESCRIPTION= Ubuntu 12.04.4 LTS
  - `mpif90 -v`

    mpif90 for MPICH version 3.0.3
    ifort version 13.0.0
- Mageia on Intel Core i7-4765T (2GHz) with 8GB RAM
  - `uname -a`

    Linux 3.10.28-desktop-1.mga3 #1 SMP Sat Feb 1 16:15:10 UTC 2014 x86_64 x86_64 x86_64 GNU/Linux
  - `lsb_release -a`

    Distributor ID: Mageia

Description: Mageia 3
Release: 3
Codename: thornicroft

– `mpif90 -v`
mpif90 for MPICH2 version 1.2.1
ifort version 14.0.1

6 Examples

These examples are located in `MO-IPT/data/`.

- **sample_1:** Model calculation of the doped two-orbital degenerate Hubbard Model for density-density type interaction at $T = 0$. The $U = 1.5$, $J_H = 0$, and the total filling, $n_{tot} = 1.6$. The bare density of states is a Gaussian (Hypercubic lattice). The relevant files are in `data/sample_1`.

- **sample_2:** Model calculation of the half-filled non-degenerate two-orbital Hubbard model for density-density type interactions. The system is half-filled ($n_{tot} = 2$) but not p-h symmetric. The $U = 1.5$ and $J_H = 0$. The relevant files are in `data/sample_2`.

- **sample_3:** Real material calculation for $SrVO_3$ at $T = 0$. The DFT input, $H_0(k)$, has been obtained through WIEN2K and Wannier90 through standard procedures. The $U = 1.2$ and $J_H = 0.1$. The relevant files are in `data/sample_3`.

- **sample_4:** Real material calculation for $SrVO_3$ at $T = 0.1eV$. The DFT input, $H_0(k)$, has been obtained through WIEN2K and Wannier90 through standard procedures. The relevant files are in `data/sample_4`.

- **sample_5:** Model calculation of the half-filled, p-h symmetric two-orbital Hubbard model at $U = 1.5$, and $J_H = 0$ on a 2-D square lattice with 120 k-points along each direction. The relevant files are in `data/sample_5`.

7 Flowchart

The full flowchart of the LDA+DMFT method is displayed in `docs/flowchart.pdf`. A description of the symbols may be found in Dasari et al [].