

EDIPack2: interoperable Lanczos-based solver for generic quantum impurity problems

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Abstract

Keywords: Exact diagonalization, Quantum Impurity models, Strongly correlated electrons, Dynamical Mean-Field Theory

PROGRAM SUMMARY

Program Title: EDIPack2

Licensing provisions: GPLv3

Programming language: Fortran, Python

Classification: 6.5, 7.4, 20

Required dependencies: CMake ($\geq 3.0.0$), Scifortran, MPI

Nature of problem: .

Solution method: .

1. Introduction and Motivation

A few words about the motivations who led us to develop this software, possible applications and advantages:

- * flexibility: can address generic cases including multi-orbital, superconducting or spin-non-conserving regimes

- * zero and low finite temperatures

- * direct access to (well approximated) analytic dynamical functions

- * direct access to impurity Fock space quantities

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2. Structure and derived software

EDIPack2 is a modular library which contains three principal structures. At the core is the exact diagonalization solver: EDIPack2 . Next there is a EDIPack2ineq which extends application to the case of multiple inequivalent impurity problems. Finally, there we provide a Fortran-C interface, which enables development of additional API or inter-operability with external libraries.

- **EDIPack2.** This constitutes the building block of the whole software. This part implement the with the Lanczos-based solver for generic quantum impurity systems encoding different symmetries, i.e. quantum number conservations and apt to solve multi-orbital problems, also in presence of coupling to local phonons. The EDIPack2 solver has a hierarchical and modular structure: different sections of the library communicate through a shared memory layer. The top module of the library is EDIPACK2 which, once loaded, enables access to the Fortran API in terms of suitable procedures to initialize, execute and finalize the solver or to retrieve internal quantities while making opaque to the user the internal structure of the library. A detailed presentation of the library can be found in Sec.4.
- **EDIPack2ineq.** This part of the software, leveraging on the object oriented concepts available in modern Fortran, aims to extend the EDIPack2 library to the case of multiple inequivalent and independent impurity problems. This is particularly useful while using EDIPack2 as a solver for DMFT in presence of unit cells with inequivalent atoms, for systems with somehow broken translational symmetry (e.g. heterostructures, large supercells, etc.).
- **EDIPack2 C-bindings.** EDIPack2 includes a single module implementing a Fortran-C interface of the main library procedures. The module is developed around the implicit ISO_C_BINDING capabilities of the most recent Fortran distributions, which enable to translate Fortran procedures directly to C. In order to overcome all the difficulties related to the internal structure of the library, we interfaced all and just the procedures and the variables exposed to the user. This module aims to foster interoperability of EDIPack2 with different third party softwares as well as to support development of additional API.
- **EDIPy2.** This is a simple Python module which provides Python API to the EDIPack2 Fortran library. This interface is built around the Python support to C-types, which allows to import the dynamic C-binding library generated upon building EDIPack2 . The module contains a specific class, whose methods mirrors through duck-typing all the available procedures of EDIPack2 as well as it gives access to relevant shared control variables.
- **EDIPack2Triqs.** This is a thin interface layer from EDIPack2 to Triqs, built around the Python API of the EDIPack2 library. The exact diagonalization solver is encapsulated in a dedicated class, containing the necessary methods to initialize and run a single instance of the solver. The interface also includes a specific class encompassing the effective discretized bath structure as well as their optimization methods.

3. Installation

The installation of EDIPack2 is available through CMake which ensures multi-platforms compability and dependencies resolution. The software builds into two distinct libraries. The main one is `libedipack.a` which, alongside the generated Fortan modules, wraps the EDIPack2 software possibly including support for inequivalent impurities. A second dynamic library, `libedipack.cbinding.so`, enables interoperability through specific bindings to the C programming language.

3.1. Dependencies

EDIPack2 essentially depends on two external libraries.

- **SciFortran:** an open-source Fortran library to support mathematical and scientific software development.

- **MPI** (optional): a distributed memory parallel communication layer with support to modern Fortran compiler.

SciFortran provides a solid development platform enabling access to many algorithms and functions, including standard linear algebra operations and high-performance Lanczos based algorithms. This greatly reduces code clutter and development time. The use of distributed memory parallel environment, although optional, is required to access scalable parallel diagonalization algorithms which speed up calculations for large dimensional systems.

3.2. Build and Install

3.2.1. Source

The software can be installed from source as follows. The source can be retrieved directly from its GitHub repository, for instance using:

```
1 git clone https://github.com/edipack/EDIPack2.0 EDIPack2
```

Then, assuming to be in the software directory, a conventional out-of-source building is performed using two different compilations backends.

- **GNU Make**

This is the default CMake workflow:

```
1 mkdir build
2 cd build
3 cmake ..
4 make -j
5 make install
```

- **Ninja**

An alternative workflow employs the Ninja building backend with Fortran support. Ninja is generally faster and automatically supports multi-threaded building:

```
1 mkdir build
2 cd build
3 cmake -GNinja ..
4 ninja
5 ninja install
```

The CMake configurations can be further tuned using the following variables:

Option	Scope	Value
-DPREFIX	Install directory	~/opt/EDIPack2/TAG/PLAT/BRANCH
-DUSE_MPI	MPI support	True/False
-DWITH_INEQ	Inequivalent impurities support	True/False
-DVERBOSE	Verbose CMake output	True/False
-DBUILD_TYPE	Compilation flags	RELEASE/TESTING/DEBUG/AGGRESSIVE

The default target builds and install either the main library and the C-binding. However, a specific building for each library is available specifying the required target. A recap message is printed at the end of the CMake configuration step.

3.2.2. Anaconda

As an alternative we provide for both Linux and OSX systems installation through Anaconda packages into a virtual environment containing Python (> 3.10).

The Conda package installation procedure reads:

```
1 conda create -n edipack
2 conda activate edipack
3 conda install -c conda-forge -c edipack edipack2
```

which installs a bundle of Scifor and EDIpack2 libraries together with specific `pkg-config` configurations files which can be used to retrieve compilation and linking flags.

3.3. OS Loading

In order to avoid possible conflicts or require administrative privileges, the building step results get installed by default in a user home directory, specified by the CMake variable `PREFIX`. In doing so, however, one misses the chance of automatic loading into the operative system.

We offer different strategies to perform this action:

1. A CMake generated configuration file for environment module which allows to load and unload the library at any time. This is preferred solution for HPC systems.
2. A CMake generated bash script to be sourced (once or permanently) in any shell session to add EDIpack2 library to the default environment.
3. A CMake generated `pkg-config` configuration file to be added in the `pkg-config` path itself.

An automatically generated recap message with all instructions is generated at the end of the installation procedure.

3.4. Python API

3.4.1. Build from source

EDIpy2, i.e. the Python API of EDIpack2, is available as a stand-alone module which depends on both EDIpack2 and SciFortran. The package can be obtained from the repository [EDIpy2](#).

```
1 git clone https://github.com/edipack/EDIpy2 EDIpy2
2 cd EDIpy2
3 pip install .
```

In some more recent Python distribution the flag `--break-system-packages` might be required to complete installation or a virtual environment should be used instead.

3.4.2. Anaconda

As for EDIpack2, also the Python API in EDIpy2 are available through Anaconda packaging. In this case the resolution of the dependencies is taken care from Conda itself:

```
1 conda create -n edipack
2 conda activate edipack
3 conda install -c conda-forge -c edipack edipack2
```

3.5. TRIQS interface

A purely Python EDIpack2 to Triqs interface is available, leveraging on the C-bindings and Python API. The corresponding module depends on EDIpack2 (which ultimately depends on SciFortran) and Triqs. Assuming the two software are correctly installed in the OS, the EDIpack2Triqs interface is installed as follows:

```
1 git clone https://github.com/krivenko/edipack2triqs
2 cd edipack2triqs
3 pip install .
```

4. Implementation

Here we present an overview of the implementation of the different parts of the EDIpack2 library.

4.1. The quantum impurity problem

We consider a general quantum impurity problem defined by the following Hamiltonian:

$$\hat{H} = \hat{H}_{imp} + \hat{H}_{bath} + \hat{H}_{hyb} + \hat{H}_{ph} + \hat{H}_{e-ph}$$

which describes a multi-orbital interacting quantum impurity coupled to an electronic bath and to local, i.e. Holstein, phonons. We assume for the moment that no particular symmetry holds. The impurity part of the Hamiltonian reads:

$$\begin{aligned} \hat{H}_{imp} &= \hat{H}_{imp}^0 + \hat{H}_{imp}^{int} \\ \hat{H}_{imp}^0 &= \sum_{\alpha\beta\sigma\sigma'} h_{\alpha\beta\sigma\sigma'}^0 d_{\alpha\sigma}^+ d_{\beta\sigma'} \\ \hat{H}_{imp}^{int} &= U \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow} + U' \sum_{\alpha \neq \beta} n_{\alpha\uparrow} n_{\beta\downarrow} + (U' - J) \sum_{\alpha < \beta, \sigma} n_{\alpha\sigma} n_{\beta\sigma} \\ &\quad - J_X \sum_{\alpha \neq \beta} d_{\alpha\uparrow}^+ d_{\alpha\downarrow} d_{\beta\downarrow}^+ d_{\beta\uparrow} + J_P \sum_{\alpha \neq \beta} d_{\alpha\uparrow}^+ d_{\alpha\downarrow}^+ d_{\beta\downarrow} d_{\beta\uparrow} \end{aligned} \quad (1)$$

where $d_{\alpha\sigma}$ ($d_{\alpha\sigma}^+$) are the destruction (creation) second-quantization operators for impurity electrons in the orbital $\alpha = 1, \dots, N_\alpha$, with N_α the number of orbitals, with spin $\sigma = \uparrow, \downarrow$ and whose occupation is described by the operator $n_{\alpha\sigma} = d_{\alpha\sigma}^+ d_{\alpha\sigma}$. The non-interacting internal structure of the impurity is described by the $h_{\alpha\beta\sigma\sigma'}^0$ matrix. \hat{H}_{imp}^{int} describes the local multi-orbital interaction¹ which, for simplicity, we take as a generalized Hubbard-Kanamori form. The first three terms represent the density-density part of the interaction, where U is the local intra-orbital Coulomb repulsion, U' the inter-orbital one and J the Hund's coupling¹. The remaining two terms are, respectively, the spin-exchange and pair-hopping which we considered with their respective independent couplings J_X and J_P . In the case $N_\alpha = 3$ a fully symmetric $SU(3)_{orbital} \times SU(2)_{spin} \times U(1)_{charge}$ form of the interaction is obtained by setting $U' = U - 2J$ and $J_X = J_P = J$ ¹. Different choices, preserving part of the combined symmetry group, can be made for other values of N_α ¹.

The bath part and its coupling to the impurity has the form:

$$\begin{aligned} \hat{H}_{bath} &= \sum_p \sum_{\alpha\beta\sigma\sigma'} h_{\alpha\beta\sigma\sigma'}^p a_{p\alpha\sigma}^+ a_{p\beta\sigma'} \\ \hat{H}_{hyb} &= \sum_p \sum_{\alpha\beta\sigma\sigma'} V_{\alpha\beta\sigma\sigma'}^p d_{\alpha\sigma}^+ a_{p\beta\sigma'} + H.c. \end{aligned} \quad (2)$$

where $p = 1, \dots, N_{bath}$ is an index running over a finite number of bath elements, $a_{p\alpha\sigma}$ ($a_{p\alpha\sigma}^+$) are the destruction (creation) operators for the bath electrons with index p , with orbital α and spin σ . The properties of each bath level are described by the matrices $h_{\alpha\beta\sigma\sigma'}^p$. As such any bath element can be composed of several electronic levels according the bath topology, which will be discussed further in the following. Each bath level couples to the impurity with an amplitude $V_{\alpha\beta\sigma\sigma'}^p$ which we allow to couple different orbital and opposite spins.

Finally, the electron-phonon part of the quantum impurity problems is described by the Hamiltonian terms:

$$\begin{aligned} \hat{H}_{ph} &= \sum_q \omega_{0q} b_q^+ b_q \\ \hat{H}_{e-ph} &= \sum_q \sum_{\alpha\beta\sigma} g_{\alpha\beta} d_{\alpha\sigma}^+ d_{\beta\sigma} (b_q + b_q^+) \end{aligned} \quad (3)$$

where $q = 1, \dots, N_q$ indexes the number of local phonons, b_q (b_q^+) are the destruction (creation) operators for the phonon q with frequency ω_{0q} . The matrix $g_{\alpha\beta}$ expresses the electron-phonon coupling. Although feasible, dealing with more than one phonon mode becomes quickly computationally very demanding, thus in the rest of this work we shall consider $N_q = 1$.

In the following we consider a bath discretized into a number of bath degrees of freedom and a finite number of available phonons, to cut-off the unbounded dimensions of the local phonons Hilbert space.

More specifically, we consider a system composed of $N_{imp} = 1$ impurities, i.e. a single impurity problem, N_{bath} bath elements and N_{ph} phonons. The size of the system is determined by the number of phonons (fixed) and that of *electronic* levels, i.e. levels with a local electronic Hilbert space $\mathcal{H}_e = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$. Due to its internal structure, the single impurity contains $N_i = N_\alpha$ electronic levels. The total number of levels is then determined by the electronic levels in the bath N_b . This is a function of the bath topology and N_{bath} , i.e. the number of bath elements. In the simplest case each bath element corresponds to an independent electronic levels coupled to the impurity, thus $N_b \equiv N_{bath}$. We indicate with $N_s = N_i + N_b$ the total number of electronic levels.

4.2. The Fock basis states

The Fock space of the quantum impurity problems is defined as $\mathcal{F} = \mathcal{F}_e \otimes \mathcal{F}_{ph}$, with $\mathcal{F}_e = \bigoplus_{n=0}^{N_s} S_- \mathcal{H}_e^{\otimes n}$ the electronic Fock space, $\mathcal{F}_{ph} = \bigoplus_{n=0}^{N_q} S_+ \mathcal{H}_{ph}^{\otimes n}$ the phonon Fock space, $\mathcal{H}_{ph} = \{|0\rangle, |1\rangle, \dots, |N_{ph}\rangle\}$ is the local phonon Hilbert space and (S_-) S_+ the (anti-)symmetrization operator. The total dimension of the Fock space is $D = D_e \cdot D_{ph} = 4^{N_s} \cdot (N_{ph} + 1)$ making the exponential growth with the number of electron levels transparent. The quantum states in the space \mathcal{F} are naturally represented in terms of occupation number formalism of the second quantization, i.e. the Fock basis. For a system of N_s electrons each Fock state reads $|p\rangle|\vec{n}\rangle$ with $|\vec{n}\rangle = |\vec{n}_\uparrow\rangle|\vec{n}_\downarrow\rangle = |n_{1\uparrow}, \dots, n_{N_s\uparrow}, n_{1\downarrow}, \dots, n_{N_s\downarrow}\rangle$, where $p = 1, \dots, N_{ph}$ is the number of local phonons while $n_{a\sigma} = 0, 1$ signals the absence or the presence of an electron with spin σ at the level a . Remarkably, the electronic part of the Fock state $|\vec{n}\rangle$ is represented as a string of zeros and ones of length $2N_s$. Thus, any such state can be encoded in a computer using a sequence of $2N_s$ bits or, analogously, as a given integer $I = 0, \dots, 2^{2N_s} - 1$ so that $|\vec{n}\rangle = |I\rangle$. Together with the basis states one defines destruction and creation operators, respectively $c_{a\sigma}$ and $c_{a\sigma}^+$, which acts on the Fock space as: $|\vec{n}\rangle$ as:

$$c_{a\sigma}|\vec{n}\rangle = \begin{cases} (-1)^{\#_{a\sigma}} |\dots, n_{a\sigma}-1, \dots\rangle & \text{if } n_{a\sigma}=1 \\ 0 & \text{otherwise} \end{cases}; \quad c_{a\sigma}^+|\vec{n}\rangle = \begin{cases} (-1)^{\#_{a\sigma}} |\dots, n_{a\sigma}+1, \dots\rangle & \text{if } n_{a\sigma}=0 \\ 0 & \text{otherwise} \end{cases}$$

where $\#_{a\sigma} = \sum_{b\sigma' < a\sigma} n_{b\sigma'}$ takes care of the fermionic sign imposed by Pauli principle.

4.3. Conserved quantum numbers

In order to circumvent the exponential scaling of the dimensions of the problem scales it is necessary to take into account suitable symmetries. Indeed, considering operators \mathcal{Q} such that $[H, \mathcal{Q}] = 0$ reduces of the Fock space into several symmetry sectors labelled by given quantum numbers \vec{Q} . In the context of quantum impurity problems two symmetries are often considered: i) conservation of the total occupation N and ii) the conservation of the total magnetization S_z . Although the total spin operator S^2 can also be conserved, the difficult implementation and the marginal gain makes it often non convenient to include this symmetry.

In EDIPack2 we consider three different cases:

- **normal:** $\vec{Q} = [N, S_z] \equiv [N_\uparrow, N_\downarrow]$
- **superc:** $\vec{Q} = S_z$
- **nonsu2:** $\vec{Q} = N$

The **normal** case consider independent conservation of the total occupation N and the total magnetization S_z or, equivalently, the total number of electrons with spin up N_\uparrow and down N_\downarrow . Optionally, we consider the case in which the symmetry applies separately for each orbital and spin, i.e. $\vec{N}_\sigma = [N_\sigma^1, \dots, N_\sigma^{N_\alpha}]$. This special case has been extensively discussed in ? so it won't be covered in this work.

The **superc** case deals with the conservation of the total magnetization only, so that total charge may not be conserved. This case includes a description of *s*-wave superconductivity, featuring intra- and inter-orbital components.

Finally, the **nonsu2** case consider the conservation of the total charge, whereas the spin symmetry group is not fully conserved. Although there many possible realization of this scenario, this particularly applies to the presence of local spin-orbit coupling $\vec{L} \cdot \vec{S}$, the emergence of in-plane spin ordering[?] or in-plane spin-triplet exciton condensation^{???}.

From a computational point of view the construction of a symmetry sector corresponds to the determination of a injective map $\mathcal{M} : \mathcal{S}_{\vec{Q}} \rightarrow \mathcal{F}$ relating the states $|i\rangle$ belonging to the sector $\mathcal{S}_{\vec{Q}}$ to the states $|I\rangle$ in the Fock space. Operatively, the map corresponds to an integer rank-1 array of dimension $D_{\mathcal{S}}$ which is the *dimension* of the sector. According to the previously introduced symmetries we have:

- **normal:** $D_{\mathcal{S}} = \binom{N_s}{N_{\uparrow}} \binom{N_s}{N_{\downarrow}}$
- **superc:** $D_{\mathcal{S}} = \sum_m 2^{N_s - S_z - 2m} \binom{N_s}{N_s - S_z - 2m} \binom{S_z + 2m}{m}$
- **nonsu2:** $D_{\mathcal{S}} = \binom{2N_s}{N}$

The **normal** case requires a brief remark. Because of the independent conservation of N_{\uparrow} and N_{\downarrow} , the sector can be further factorized into $\mathcal{S}_{\vec{Q}} = \mathcal{S}_{N_{\uparrow}} \otimes \mathcal{S}_{N_{\downarrow}}$ and, correspondingly, the sector map reads $\mathcal{M} = \mathcal{M}_{\uparrow} \otimes \mathcal{M}_{\downarrow}$. As such, each state $|i\rangle = |i_{\uparrow}\rangle |i_{\downarrow}\rangle$ of the sector is labelled by two integers $[i_{\uparrow}, i_{\downarrow}]$, $i_{\sigma} = 1, \dots, D_{\mathcal{S}_{\sigma}}$ such that $i = i_{\uparrow} + i_{\downarrow} D_{\mathcal{S}_{\downarrow}}$. The map \mathcal{M} connects any such state to a Fock state $|I\rangle = |I_{\uparrow}\rangle |I_{\downarrow}\rangle$ labelled by two integers $[I_{\uparrow}, I_{\downarrow}]$ as $I = I_{\uparrow} + I_{\downarrow} 2^{N_s}$. For a thorough discussion about Fock basis organization in this case see [?].

The symmetry sector reduction of the Fock space induces a block digonal form to the Hamiltonian matrix. Each block, labelled by a value of the quantum numbers \vec{Q} has dimension $D_{\mathcal{S}(\vec{Q})}$. The sector Hamiltonian matrix $H_{\mathcal{S}}$ is represented in the basis $|i\rangle \in \mathcal{S}_{\vec{Q}}$ as a sparse matrix. In the **normal** case $H_{\mathcal{S}}$ takes a particularly symmetric form thanks to the product structure of the sector and its map[?]. The analysis of the spectrum is then reconducted to the inspection of the Hamiltonian in each symmetry sector. Should particular constraint holds the search can be limited to only particular sector, further reducing the computational cost.

Although the sectors have dimensions much smaller than the full Fock space, for large systems storing the Hamiltonian matrix in the memory can still be highly inefficient. In such cases, Krylov or Lanczos methods²⁻⁵ can be implemented using a storage-free algorithm, performing the necessary linear operations on-the-fly. This solution has generally a negative impact on the execution time, however this can be well compensated by scaling in a distributed parallel framework.

4.4. Krylov based Diagonalization

4.5. Dynamical correlation functions

4.6. Observables

4.7. Reduced impurity density matrix

4.8. Bath parametrization

4.9. Bath Optimization

4.10. Input/Output

5. Inequivalent impurities

6. C-bindings

7. Python API

8. Triqs interface

9. Usage

9.1. *Bethe lattice DMFT (Fortran API)*

9.2. *Attractive Hubbard model (Python API)*

9.3. *Multi-orbital Hubbard (Triqs)*

10. Conclusions

Acknowledgements

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