EDIpack2.0plus Triqs interface

L. Crippa, I. Krivenko, S. Giuli, G. Bellomia, ..., A. Amaricci[a,*]

[a] *CNR-IOM, Istituto Officina dei Materiali, Consiglio Nazionale delle Ricerche, Via Bonomea 265, 34136 Trieste, Italy*

Abstract

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

PROGRAM SUMMARY

Program Title: EDIpack2.0
Licensing provisions: GPLv3
Programming language: Fortran, Python
Classification: 6.5, 7.4, 20
Required dependencies: CMake (>= 3.0.0), Scifortran, MPI
Nature of problem:.
Solution method: .

*Corresponding author.
E-mail address: amaricci@iom.cnr.it

5.1. The quantum impurity problem

We consider a system of N_s electronic levels. A portion N_α of them, i.e. the impurity levels, interact via a local repulsion, while the remaining $N_s - N_\alpha$, i.e. the *bath* levels, are non-interacting. In a typical setup the impurity levels are independently coupled to a set of N_b electronic levels, so that the total number is $N_s = N_\alpha(N_b + 1)$. Other choices for the bath topology are possible, which entail a different counting of the total levels. The Hamiltonian of the electronic system we consider has the form:

$$\begin{aligned}
\hat{H}^e =& \hat{H}^0 + \hat{H}^{int} \\
\hat{H}^0 =& \sum_{\alpha\beta\sigma} H^{loc}_{\alpha\beta\sigma} d^+_{\alpha\sigma} d_{\beta\sigma} + \\
& \sum_{\nu\alpha\beta\sigma} h^\nu_{\alpha\beta\sigma} a^+_{\nu\alpha\sigma} a_{\nu\beta\sigma} + \sum_{\nu\alpha\sigma} V^\nu_{\alpha\sigma} d^+_{\alpha\sigma} a_{\nu\alpha\sigma} + H.c. \\
\hat{H}^{int} =& U \sum_\alpha n_{\alpha\uparrow} n_{\alpha\downarrow} + U' \sum_{\alpha\neq\beta} n_{\alpha\uparrow} n_{\beta\downarrow} + (U' - J) \sum_{\alpha<\beta,\sigma} n_{\alpha\sigma} n_{\beta\sigma} - \\
& J_X \sum_{\alpha\neq\beta} d^+_{\alpha\uparrow} d_{\alpha\downarrow} d^+_{\beta\downarrow} d_{\beta\uparrow} + J_P \sum_{\alpha\neq\beta} d^+_{\alpha\uparrow} d^+_{\alpha\downarrow} d_{\beta\downarrow} d_{\beta\uparrow}
\end{aligned} \tag{1}$$

where $a_{\alpha\sigma}$, $d_{\alpha\sigma}$ ($a^+_{\alpha\sigma}$, $d^+_{\alpha\sigma}$) are, respectively, the destruction (creation) operators for the bath and impurity electrons with orbital α and spin σ, $n_{\alpha\sigma} = d^+_{\alpha\sigma} d_{\alpha\sigma}$. The term $H^{loc}_{\alpha\beta\sigma}$ is the non-interacting part of the impurity Hamiltonian, $h^\nu_{\alpha\beta\sigma}$ and $V^\nu_{\alpha\sigma}$ are, respectively, the local Hamiltonian and the impurity hybridization of the $\nu-$th bath level. Finally, $\hat{H}^{int}$ is the local multi-orbital interaction [1]. The first three terms represent the density-density part of the interaction, while the remaining two are, respectively, the spin-exchange and pair-hopping terms. U is the local Coulomb interaction strength, J is the Hund's coupling [1]. We introduced independent coupling controlling the spin-exchange and pair-hopping terms, respectively J_X and J_P. The fully symmetric Kanamori interaction is obtained setting $U' = U - 2J$ and $J_X = J_P = J$ [1].

5.2. The basis states

A natural representation of the basis states for the Fock space $\mathcal{F}_e$ is obtained in the occupation number formalism of second quantization. The *Fock basis* for a finite system of N_s electrons is composed of states of the form $|\vec{n}\rangle = |n_{1\uparrow}, \ldots, n_{N_s\uparrow}, n_{1\downarrow}, \ldots, n_{N_s\downarrow}\rangle$, where each element $n_{a\sigma} = 0, 1$ describes the absence or the presence of an electron with spin σ at the level a. In conjunction with the basis states, we introduce the non-Hermitian, anti-commuting, annihilation and creation operators $c_{a\sigma}$ and $c^+_{a\sigma}$, respectively. These operators act on the states $|\vec{n}\rangle$ as:

$$c_{a\sigma}|\vec{n}\rangle = \begin{cases} (-1)^{\#_{a\sigma}} |\ldots, n_{a\sigma} - 1, \ldots\rangle & \text{if } n_{a\sigma} = 1 \\ 0 & \text{otherwise} \end{cases}; \tag{2}$$

$$c^+_{a\sigma}|\vec{n}\rangle = \begin{cases} (-1)^{\#_{a\sigma}} |\ldots, n_{a\sigma} + 1, \ldots\rangle & \text{if } n_{a\sigma} = 0 \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

with $\#_{a\sigma} = \sum_{b\sigma' < a\sigma} n_{b\sigma'}$. Thus, each state is represented as a string of zeros and ones, i.e. the binary decomposition of a given integer number I. Using the identification $|\vec{n}\rangle = |I\rangle$, with $I = 0, \ldots, 2^{2N_s} - 1$, each state in the Fock space can be encoded in a computer using a sequence of $2N_s$ bits or, equivalently, an integer number in a fixed representation. The exponentially growing size of the Fock space will eventually make such representation unpractical. A solution is obtained by decomposing each state according to the existing QNs. For a given set $[\vec{N}_\uparrow, \vec{N}_\downarrow]$ of QNs we then have:

$$\begin{aligned}
|\vec{n}\rangle =& \prod_{\alpha=1}^{N_{ud}} \prod_{\sigma=\uparrow\downarrow} |n_1 \ldots n_{N_{bit}}\rangle_{\alpha\sigma} \\
=& \begin{cases} |\vec{n}_\uparrow\rangle |\vec{n}_\downarrow\rangle, \text{ if } N_{ud} = 1 \\ |\vec{n}_{1\uparrow}\rangle \cdots |\vec{n}_{N_{ud}\uparrow}\rangle |\vec{n}_{1\downarrow}\rangle \cdots |\vec{n}_{N_{ud}\downarrow}\rangle, \text{ if } N_{ud} = N_\alpha \end{cases}
\end{aligned} \tag{4}$$

so that, if the total number of electrons with spin $\uparrow$ and $\downarrow$ is conserved, any state is identified by two binary sequences of $N_{bit} = N_s$ bits, one per spin orientation. Alternatively, if the number of electrons with spin $\uparrow$ and $\downarrow$ per orbital is conserved, the states are decomposed into two sets of binary sequences (one set per spin orientation), each sequence being made of $N_{bit} = N_s/N_\alpha$ bits. Each binary sequence is associated to a suitable tuple of integer numbers, univocally identifying the Fock state: $I \to [\vec{I}_\uparrow, \vec{I}_\downarrow]$, where $I = 0, \dots, 2^{2N_s} - 1$ and $\vec{I}_\sigma = [I_{1\sigma}, \dots, I_{N_{ud}\sigma}]$ with $I_{\alpha\sigma} = 0, \dots, 2^{N_{bit}} - 1$. Through such decomposition, each state can be described by the smallest bit set compatible with the conserved QNs. This setup generalizes the method introduced by Lin and Gubernatis in Ref. 2. The relation between the Fock state index I and its tuple decomposition can be easily inverted:

$$I = I_1 + \sum_{i=2}^{2N_{ud}} I_i 2^{N_{bit}(i-1)}\,, \tag{5}$$

where we rearranged the tuple as $[\vec{I}_\uparrow, \vec{I}_\downarrow] = [I_1, \dots, I_{2N_{ud}}]$.

Such organization of the Fock states is used to construct a suitable basis for the sectors $\mathcal{S}[\vec{N}_\uparrow, \vec{N}_\downarrow]$. To any given Fock state $|\vec{n}\rangle$ and its integer representation I, containing the correct bit decomposition dictated by the QNs, it is associated a state $|i\rangle$ and an integer $i = 1, \dots, D_\mathcal{S}$ through a suitable *map* $\vec{\mathcal{M}}_\mathcal{S}$. In particular, each tuple of integers identifying a Fock state belonging to $\mathcal{S}$ is associated to a new tuple specific for each sector state: $I \in \mathcal{S} = [\vec{I}_\uparrow, \vec{I}_\downarrow] \in \mathcal{S} \xrightarrow{\vec{\mathcal{M}}_\mathcal{S}} [\vec{i}_\uparrow, \vec{i}_\downarrow] = i$, where $\vec{i}_\sigma = [i_{1\sigma}, \dots, i_{N_{ud}\sigma}]$ and $i_{\alpha\sigma} = 1, \dots, D_{\alpha\sigma}$. The tuple $[\vec{i}_\uparrow, \vec{i}_\downarrow]$ univocally identifies a basis state $|i\rangle = |\vec{i}_\uparrow, \vec{i}_\downarrow\rangle$ of the sector $\mathcal{S}$, through a relation similar to (5):

$$i = i_{1\uparrow} + \sum_\sigma \sum_{l=2}^{N_{ud}} (i_{l\sigma} - 1) \prod_{\alpha=1}^{l-1} D_{\alpha\sigma} \tag{6}$$

5.3. Conserved quantum numbers

A system of N_s electrons is associated to a Fock space of the form $\mathcal{F}_e = \bigoplus_{n=0}^{N_s} S_- \mathcal{H}_e^{\otimes n}$, where $\mathcal{H}_e = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$ is the local Hilbert space of the electrons on a single level, S_- is the anti-symmetrization operator, $\bigoplus$ is the direct sum and $\bigotimes$ the tensor product. The total dimension of the Fock space $\mathcal{F}_e$ is $\dim(\mathcal{H}_e)^{N_s} = 4^{N_s} = 2^{2N_s}$.

The solution of the eigenvalue problem for H_e is simplified by taking into account the existence of conserved quantities. The Hamiltonian (1) conserves the total charge $\hat{N}$ and the spin component $\hat{S}_z$, as long as we assume that no terms breaking the particle number or spin conservation are present, e.g. local spin-orbital coupling, in-plane magnetic field, superconducting order, etc. The conservation of $\hat{N}$ and $\hat{S}_z$ can be conveniently re-expressed in terms of conserved number of electrons with spin $\uparrow$ and $\downarrow$, i.e. $\hat{N}_\uparrow$, $\hat{N}_\downarrow$. Moreover, if the terms H^{loc} and h are diagonal and we consider only the density-density part of the interaction, i.e. $J_X = J_P = 0$, the number of electrons with spin $\uparrow$ and $\downarrow$ is conserved *per orbital*, i.e. $\hat{N}^m_\uparrow$, $\hat{N}^m_\downarrow$, where $m = 1, \dots, N_\alpha$.

In order to formally unify the treatment of these two cases we introduce some convenient parameters, namely $N_{ud} = 1$ (N_α) and $N_{bit} = N_s$ (N_s/N_α) for conserved total (orbital resolved) number of electrons with spin $\uparrow$ and $\downarrow$. The first corresponds to the number of conserved operators per spin, the latter indicates the number of electronic levels per spin (spin and orbital). In the following section we will give a more precise meaning to N_{bit}.

In the rest of this work we will indicate the set of conserved quantum numbers (QN)s with the tuple $[\vec{N}_\uparrow, \vec{N}_\downarrow]$, where ($\sigma = \uparrow, \downarrow$):

$$\vec{N}_\sigma = \begin{cases} N_{1\sigma} \equiv N_\sigma, & \text{if } N_{ud} = 1 \\ [N_{1\sigma}, \dots, N_{N_\alpha\sigma}], & \text{if } N_{ud} = N_\alpha \end{cases} \tag{7}$$

Note that for $N_{ud} = 1$ we identified the single component $N_{1\sigma}$ of the vector $\vec{N}_\sigma$ with the total number of electrons with spin σ, i.e. N_σ.

In presence of a set of conserved QNs, the Fock space decomposes into a number of sub-spaces of reduced dimension, each corresponding to a given value of the QNs tuple. We indicate each sub-space with the term *sector* and the symbol $\mathcal{S}[\vec{N}_\uparrow, \vec{N}_\downarrow]$, or just $\mathcal{S}$ where no confusion arises. The dimension of each sector is given by the number of ways we can arrange $N_{\alpha\sigma}$ elements into N_{bit} positions, i.e.:

$$\begin{aligned}\dim\left(\mathcal{S}[\vec{N}_\uparrow, \vec{N}_\downarrow]\right) &= \prod_{\alpha=1}^{N_{ud}} \binom{N_{bit}}{N_{\alpha\uparrow}} \prod_{\alpha=1}^{N_{ud}} \binom{N_{bit}}{N_{\alpha\downarrow}} \\ &\equiv \prod_{\alpha=1}^{N_{ud}} D_{\alpha\uparrow} \prod_{\alpha=1}^{N_{ud}} D_{\alpha\downarrow} \stackrel{\text{def}}{=} D_\uparrow D_\downarrow \equiv D_{\mathcal{S}}\end{aligned} \tag{8}$$

where we introduced the symbols D_σ and $D_{\alpha\sigma}$ to indicate, respectively, the dimension of total and orbital spin-subspace associated to the given set of QNs. Note that $D_\sigma \equiv D_{1,\sigma}$ for $N_{ud} = 1$.

5.4. Krylov based Diagonalization

The matrix representing the system Hamiltonian in the Fock space has a block-diagonal structure in presence of a given set of conserved QNs. Each block corresponds to the Hamiltonian of a sector $\mathcal{S}[\vec{N}_\uparrow, \vec{N}_\downarrow]$. The analysis of the spectrum, thus, reduces to the recursive analysis of the sector Hamiltonians. In each sector, the Hamiltonian of the system has the following general form:

$$H^e_{\mathcal{S}} = H_d + H_\uparrow \otimes \mathbb{I}_\downarrow + \mathbb{I}_\uparrow \otimes H_\downarrow + H_{nd}\,. \tag{9}$$

H_d is a diagonal term containing the local part of the Hamiltonian, including the density-density terms of the interaction. The H_σ components describe all the hopping processes of the electrons with spin $\sigma =\uparrow,\downarrow$. Finally the term H_{nd} contains all the remaining non-diagonal elements which do not fit in the previous two components, e.g. the spin-exchange and pair-hopping interaction terms. If the QNs are conserved per orbital, i.e. if $H_{nd} \equiv 0$ and no inter-orbital local hopping terms are present, each H_σ further splits into a sum of smaller terms:

$$H_\sigma = \sum_{\alpha=1}^{N_\alpha} \mathbb{I}_{1\sigma} \otimes \cdots \otimes H_{\alpha\sigma} \otimes \cdots \otimes \mathbb{I}_{N_\alpha\sigma}$$

Each term of the Hamiltonian matrix is constructed independently iterating over one or more components of the sector basis states. For example, the construction of the matrices $H_{\alpha\sigma}$ only involve iterations over the components $|i_{\alpha\sigma}\rangle$ of the sector basis. In general we have:

$$\begin{aligned}\langle \vec{i}_\uparrow \vec{i}_\downarrow | H^e_{\mathcal{S}} | \vec{j}_\uparrow \vec{j}_\downarrow \rangle =& \langle \vec{i}_\uparrow \vec{i}_\downarrow | H_d + H_\uparrow \otimes \mathbb{I}_\downarrow + \mathbb{I}_\uparrow \otimes H_\downarrow + H_{nd} | \vec{j}_\uparrow \vec{j}_\downarrow \rangle \\ =& \langle \vec{i}_\uparrow \vec{i}_\downarrow | H_d | \vec{i}_\uparrow \vec{i}_\downarrow \rangle + \\ & \langle \vec{i}_\uparrow | H_\uparrow | \vec{j}_\uparrow \rangle \delta_{\vec{i}_\downarrow \vec{j}_\downarrow} + \langle \vec{i}_\downarrow | H_\downarrow | \vec{j}_\downarrow \rangle \delta_{\vec{i}_\uparrow \vec{j}_\uparrow} + \\ & \langle \vec{i}_\uparrow \vec{i}_\downarrow | H_{nd} | \vec{j}_\uparrow \vec{j}_\downarrow \rangle\end{aligned} \tag{10}$$

For very large systems, storing the Hamiltonian matrix in the memory can be highly inefficient. In such cases, Krylov or Lanczos methods[2–5] 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 massively parallel framework.

5.5. Dynamical correlation functions, observables and reduced impurity density matrix

5.6. Bath parametrization

5.7. Bath χ^2 fit

5.8. Input/Output

6. EDIpy: Python API

7. edipack2triqs: a thin interface to TRIQS

8. Conclusions

Acknowledgements

References

[1] A. Georges, L. de' Medici, J. Mravlje, Strong Correlations from Hund's Coupling., Annu. Rev. Condens. Matter Phys. 45 (2013) 137–178.

[2] H. Lin, J. Gubernatis, Exact diagonalization methods for quantum systems, Computers in Physics 7 (4) (1993) 400–407. URL https://doi.org/10.1063/1.4823192

[3] C. Lanczos, An iteration method for the solution of the eigenvalue problem of linear differential and integral operators, J. Res. Natl. Bur. Stand. B 45 (1950) 255–282. doi:10.6028/jres.045.026.

[4] R. Lehoucq, D. Sorensen, C. Yang, ARPACK Users' Guide: Solution of Large-scale Eigenvalue Problems with Implicitly Restarted Arnoldi Methods, Software, Environments, Tools, Society for Industrial and Applied Mathematics, 1998. URL https://books.google.it/books?id=iMUea23N_CQC

[5] K. J. "Maschhoff, D. C. Sorensen, P_arpack: An efficient portable large scale eigenvalue package for distributed memory parallel architectures, in: J. "Waśniewski, J. Dongarra, K. Madsen, D. Olesen (Eds.), Applied Parallel Computing Industrial Computation and Optimization, Springer Berlin Heidelberg, Berlin, Heidelberg, 1996, pp. 478–486.