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Exact diagonalization library for quantum electron models☆

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ABSTRACT

We present an exact diagonalization C++ template library (EDLib) for solving quantum electron models, including the single-band finite Hubbard cluster and the multi-orbital impurity Anderson model. The observables that can be computed using EDLib are single particle Green's functions and spin–spin correlation functions. This code provides three different types of Hamiltonian matrix storage that can be chosen based on the model.

Program summary
Program Title: EDLib
Program Files doi: http://dx.doi.org/10.17632/633698b4g2.1
Licensing provisions: MIT
Programming language: C++, MPI
External routines: ARPACK-NG, ALPSCore library (Gaenko et al., 2016)
Nature of problem: The finite Hubbard and Anderson models play an essential role in the description of strongly correlated many-particle systems. These models consist of a small number of localized orbitals with Coulomb interaction between electrons and (in case of the Anderson model) non-interacting bath energy levels. The finite Hubbard cluster can be used to study molecular magnets, such as Mn_{12}, Fe_4, Mn_4, and V_{15}, which are currently of interest due to their potential for use in novel technologies such as molecular electronics, solar energy harvesting, thermoelectrics, sensing, and other applications (Sakon et al., 2004; Accorsi et al., 2006; Friedman et al., 1996) [1–3]. The Anderson model can be used to study impurities adsorbed on surfaces (Iskakov et al., 2015) [4] and appears as an impurity model in the Dynamic Mean Field Theory (Georges et al., 1996) [5].
Solution method: The OpenMP and MPI parallelized versions of the finite temperature Lanczos diagonalization method are used to diagonalize Hamiltonian matrix and to compute observables.

1. Introduction

Further progress in material science is connected with the development of appropriate theoretical concepts and methods to treat realistic modern materials and devices [1–3] taking their atomic structure, chemical composition, electronic and magnetic properties fully into account. Two of the basic quantum models for systems with strong electron–electron correlations are the Hubbard model [6] and the Anderson impurity model [7], which can be used to simulate lattice problems or an impurity in metal respectively.

At the moment, there are a number of well-developed numerical techniques one can use to solve these quantum electron models such as continuous-time quantum Monte-Carlo method [8]; numerical renormalization group [9]; density matrix renormalization group [10]; and configuration interaction methods [11]. For instance, many interesting and promising results were obtained by using QMC-type methods such as continuous-time quantum Monte Carlo method [12]. Since the main computational task is a sampling of a complex integral, these methods are ideally suited for parallelization. However, there is a fundamental problem of the QMC solvers called the sign problem, which can occur for models with a non-diagonal Coulomb interaction matrix, lattice problem away from half-filling or when the simulation temperature is rather low [13].

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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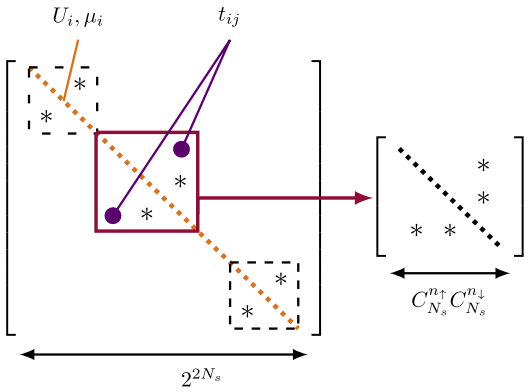

Fig. 1. Block structure of the S^z-symmetric model Hamiltonian matrix.

Alternatively, truncating the infinite Hilbert space by solving a finite lattice problem or by an infinite bath discretization with a finite set of energy levels allows one to use exact diagonalization techniques to treat the Anderson Impurity Hamiltonian. Such a method allows to diagonalize the electronic Hamiltonian for different geometries of lattice cluster or with different forms of the on-site Coulomb matrix [14,15]. Another advantage of the exact diagonalization method is that it provides a natural way to calculate real-frequency correlation functions such as one- and two-particle Green's functions at finite temperatures.

In this work, we present the parallel Exact diagonalization library for solving the eigenvalue problem of the quantum electron models on distributed-memory and shared memory computing systems.

2. Exact diagonalization of finite quantum electron models

The Hamiltonian of the many quantum electron models can be expressed as the sum of local (diagonal) term and non-diagonal hopping term as follows:

$$\mathcal{H} = \mathcal{H}_{loc} + \mathcal{H}_{hop}. \tag{1}$$

For example in case of Hubbard model [6] $\mathcal{H}_{loc} = \sum_i U_i n_{i\uparrow} n_{i\downarrow} - \sum_{i\sigma} \mu_i n_{i\sigma}$ and $\mathcal{H}_{hop} = \sum_{\langle i,j\rangle\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma}$, where U_i is Coulomb potential on site i; $\mu_i -$ chemical potential on site i; $t_{ij} -$ hopping integral between sites i, j. $c^{(\dagger)}_{i\sigma} -$ annihilation (creation) operator of electron with spin direction σ on ith site. $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma} -$ occupation number, number of electrons on the site.

The first step of exact diagonalization algorithm is to represent a Hamiltonian operator (1) as a matrix. Despite the fact that for most quantum electron models this matrix is very sparse (99% of matrix elements being zeros) the dimension still grows exponentially $M = 2^{2N_s}$ in occupation number space $|n_{1\uparrow}, \ldots, n_{N_s\uparrow} \mid n_{1\downarrow}, \ldots, n_{N_s\downarrow}\rangle$, where N_s is the number of electron levels in the studied quantum electron model. The exponential growth of basis size puts serious restriction on the problem size.

And to partially overcome this problem the symmetry properties of the particular Hamiltonian should be used. For example, for the Hubbard model there are particle and spin conservations and the matrix assumes block-diagonal form of $(N_s + 1)^2$ blocks – so called *sectors* – of much smaller dimension $M_{n_\uparrow n_\downarrow} = C^{n_\uparrow}_{N_s} \cdot C^{n_\downarrow}_{N_s}$ for a fixed total occupancy for each spin $n_\uparrow = \sum_{i=1}^{N_s} \hat{n}_{i\uparrow}$, $n_\downarrow = \sum_{i=1}^{N_s} \hat{n}_{i\downarrow}$, where C^k_n is the number of combinations of k from n elements, and N_s is the number of sites in the finite cluster. These sectors are linearly independent and can be diagonalized separately (see Fig. 1). Despite the fact that the dimension of the largest sector in general cases is smaller than the dimension of the full Hamiltonian matrix by an order of magnitude and matrix sparsity (99% of the elements are zeros for both matrices), the memory requirements still remain high enough to cause difficulties [16] and various high-performance techniques should be applied.

2.1. Exact diagonalization of the single multi-orbital impurity Anderson model

The multi-orbital impurity Anderson model can be written in the following general form:

$$\mathcal{H} = \sum_{p\sigma} \epsilon_p c^+_{p\sigma} c_{p\sigma} + \sum_{i\sigma} (\epsilon_i - \mu) n_{i\sigma} + \sum_{ip\sigma} (V_{ip} d^+_{i\sigma} c_{p\sigma} + H.c.) + \frac{1}{2} \sum_{\substack{ijkl \\ \sigma\sigma'}} U_{ijkl} d^+_{i\sigma} d^+_{j\sigma'} d_{l\sigma'} d_{k\sigma}. \tag{2}$$

Here ϵ_i and ϵ_p are energies of the impurity and bath states, $d^+_{i\sigma}$ and $c^+_{p\sigma}$ are the creation operators for impurity and surface electrons, V_{ip} is a hopping between impurity and surface states, U_{ijkl} is the Coulomb matrix element and the impurity orbital index i (j, k, l) runs over the $d-$ states. Depending on the problem we solve the bath can correspond to either an effective Weiss field (DMFT) [5] or, for instance, metallic surface states (adatom on a substrate) [4]. Since the general Coulomb interaction contains non density–density terms the local part of Hamiltonian matrix is no longer diagonal and the additional effort during parallelization is required.

3. Storage formats

3.1. Spin-resolved Hamiltonian storage format

Usually the interaction part of the Hamiltonian is diagonal and does not require additional effort to compute matrix vector product, therefore in this section we will consider the matrix representation of the hopping term of the Hamiltonian (1) only. Since the hopping

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