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Recent applications of the DMRG method

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Since its inception, the DMRG method has been a very powerful tool for the calculation of physical properties of low-dimensional strongly correlated systems. It has been adapted to obtain dynamical properties and to consider finite temperature, time-dependent problems, bosonic degrees of freedom, the treatment of classical problems and non-equilibrium systems, among others. We will briefly review the method and then concentrate on its latest developments, describing some recent successful applications. In particular we will show how the dynamical DMRG can be used together with the Dynamical Mean Field Theory (DMFT) to solve the associated impurity problem in the infinite-dimensional Hubbard model. This method is used to obtain spectral properties of strongly correlated systems. With this algorithm, more complex problems having a larger number of degrees of freedom can be considered and finite-size effects can be minimized.

Keywords: Density Matrix Renormalization; strongly correlated electrons; low dimensional systems; Dynamical Mean Field Theory

1. Introduction

The Density Matrix Renormalization Group was developed by S. White in 1992[4] and since then DMRG has proved to be a very powerful method for low dimensional interacting systems. Its remarkable accuracy can be seen for example in the spin-1 Heisenberg chain: for a system of hundreds of sites a precision of 10^{-10} for the ground state energy can be achieved. It has been applied to a great variety of systems and problems including, among others, spin chains and ladders, fermionic and bosonic systems, disordered models, impurities and molecules and 2D electrons in high magnetic fields. It has also been improved substantially in several directions like two (and three) dimensional (2D) classical systems, stochastic models, problems with phonons, quantum chemistry, field theory, the inclusion of temperature and the calculation of dynamical and time-dependent properties. Some calculations have also been performed in 2D quantum systems. These topics are treated in detail and in a pedagogical way in the book [5], where the reader can find an extensive review on DMRG. Recent reviews on DMRG can also be found in [6] and [7].

When considering finite systems, the exponential growth of degrees of freedom to be considered impose an important limitation in numerical calculations. Several

methods have been introduced in order to reduce the size of the Hilbert space to be able to reach larger systems, such as Monte Carlo, renormalization group (RG) and DMRG. Each method considers a particular criterion for keeping the relevant information. For example, in RG methods, only the lowest-lying states are kept in each building block having an excellent performance for the Kondo and Anderson impurity models (Wilson NRG)[9] but a very poor outcome for strongly correlated systems like the Hubbard model.

In the following Section we will briefly describe the standard method; in Sect. 3 we will mention some of the most important applications and extensions; in Sect.4 we describe how to calculate dynamical properties and finally, in Sect. 5 we will describe how DMRG can be used within the Dynamical Mean Field theory (DMFT) to improve the performance of this latter method.

2. Basic Facts

The DMRG allows for a systematic truncation of the Hilbert space by keeping the most probable states in describing a wave function (*e.g.* the ground state) of a larger system, instead of the lowest energy states usualy kept in previous real space renormalization techniques. The method is very well described in Ref. [8] but I shall summarize it so as to unify notations. Let's define block [**B**] as a finite chain with N_B sites, having an associated Hilbert space where operators are defined (specially the Hamiltonian in this finite chain and the operators at the ends of the block, useful for linking it to other chains or added sites). We also define an added block or site as [**a**] (see Fig. 2)

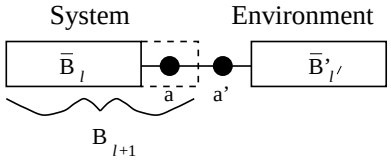

Fig. 1. A scheme of the superblock (universe) configuration for the DMRG algorithm[8].

Below we describe a general iteration of the method:

i) Define the Hamiltonian for the superblock formed by putting together two blocks [**B**] and two added sites in such a way: [**B a B' a'**] (the primes are only to indicate additional blocks, but the blocks have the same structure as the non-primed ones). In general, blocks [**B**] and [**B'**] come from the previous iteration. The total Hilbert space of this superblock is a direct product of the individual spaces corresponding to each block and the added sites. Here periodic boundary conditions can be attached between [**a'**] and [**B**] (the ends of the superblock). Diagonalize the Hamiltonian to obtain the ground state $|\psi_0\rangle$ (other states could also be kept, such

as the first excited ones: they are called target states).

ii) Construct the density matrix $\rho_{ii'} = \sum_j \psi_{0,ij}\psi_{0,i'j}$ on block [**B a**] where $\psi_{0,ij} = \langle i \otimes j|\psi_0\rangle$, the states $|i\rangle$ belonging to the Hilbert space of the block [**B a**] and the states $|j\rangle$ to the block [**B' a'**]. The density matrix considers the part [**B a**] as a system and the rest, (*i.e.* [**B' a'**]), as a statistical bath. The eigenstates of ρ with the highest eigenvalues correspond to the most probable states (or equivalently the states with higher weight) of block [**B a**] in the ground state defined in the whole superblock. These states are kept up to a certain cutoff, keeping a total of m states per block. The density matrix eigenvalues sum to unity and the truncation error, defined as the sum of the density matrix eigenvalues corresponding to discarded eigenvectors, gives a qualitative indication of the accuracy of the calculation.

iii) These states form a new reduced basis to which all the operators have to be changed and the block [**B a**] is renamed as block [**B**].

iv) A new block [**a**] is added (one site in our case) and the new superblock [**B a B' a'**] is formed as the direct product of the states of all the blocks.

v) This iteration continues until the desired length is achieved. At each step the length is $2N_B+2$ (if [**a**] consists of one site).

When more than one target state is used, *i.e* more than one state is wished to be well described, the density matrix is defined as $\rho_{ii'} = \sum_l p_l \sum_j \phi_{l,ij}\phi_{l,i'j}$, where p_l defines the probability of finding the system in the target state $|\phi_l\rangle$ (not necesseraly eigenstates of the Hamiltonian).

The method described above is usually called the *infinite-system algorithm* since the system size increases at each iteration. There is a way to increase precision at each length N called the *finite-system algorithm*. It consists of fixing the lattice size and zipping a couple of times until convergence is reached. In this case and for the block configuration [**B a a' B'**], $N = l + 1 + 1 + l'$ where l and l' are the number of sites in B and B' respectively. In this step the density matrix is used to project onto the left $l+1$ sites. In order to keep N fixed, in the next block configuration, the right block B' should be defined in $l-1$ sites such that $N = (l+1)+1+1+(l-1)'$. The operators in this smaller block should be kept from previous iterations (in some cases from the iterations for the system size with $N-2$)[5].

To calculate static properties like correlation functions one must keep the relevant operators at each step and perform the corresponding basis change and reduction, in a similar manner as done with the Hamiltonian in each block[8]. The energy and measurements are calculated in the superblock. In Ref.[12] an interpretation of the correlation functions of systems at criticality is given in terms of wave function entanglement, conjecturing a modification of DMRG for these cases that preserves the entanglement.

In connection with the above, recent work[13,14] has focused on the quantum information perspective of DMRG by calculating the von Neumann entropy of entanglement. Within this frame it can be shown that DMRG, in its present form, is not suited for calculations in dimensions higher than one.

An interesting analysis on DMRG accuracy is done in Ref. [15]. Fixed points of the DMRG and their relation to matrix product wave functions were studied in [17] and an analytic formulation combining the block renormalization group with variational and Fokker-Planck methods in [18]. The connection of the method with quantum groups and conformal field theory is treated in [19]. There are also interesting connections between the density matrix spectra and integrable models[20] via corner transfer matrices.

3. Applications and Extensions to DMRG

The number of papers using DMRG has grown enormously since its development. For example, since 1998 there have been around 80 papers using DMRG published a year. There have also been several improvements to the method and it is now used in areas that are very different to the original strongly correlated electron system field. We will only mention very briefly the main applications here and refer the reader to the reviews on the subject were most of the references are given as well as some details of the calculations [6,7]

One of the first calculations that showed the potential of the method was obtained by White and Huse [21] when calculating the spin gap in a $S = 1$ Heisenberg chain and very precise spin correlation functions and excitation energies. Several calculations were devoted to spin chains and ladders, with different values of total spin obtaining very accurate results for the excitation spectra, thermodynamics and scaling behaviour[54].

The application of DMRG to fermionic systems has been very extensive and interesting results have been obtained for one-dimensional Hubbard and t-J models and their generalizations. Bosonic degrees of freedom like phonons were introduced and applied to calculate properties of the Holstein model. Pure bosonic systems have also been calculated such as the Bose-Hubbard model. It has been generalized to 1D random and disordered systems, and applied to the random antiferromagnetic and ferromagnetic Heisenberg, including quasiperiodic exchange modulation and other systems.

A first step towards higher dimensions was the application to ladder systems (spin and fermionic ones) to study different properties like magnetization plateaus. An interesting review on the applications to some exact and analytical techniques for quantum magnetism in low dimension, including DMRG, is presented in [23]. Quite large two-dimensional systems could be reached considering several leg ladders or different sweeping algorithms in square lattices, but there's no reliable and systematic implementation of the method in 2D yet and its performance is still much poorer than in 1D. Recently, there has been an interesting approach to 2D quantum systems based on matrix product states.[13] Long-range Coulomb interactions leading to several phases have been found using DMRG for 2D electrons in high magnetic fields considering different Landau levels.

Impurity problems have been studied for example in one- and two-impurity

Kondo systems, in spin chains and in Luttinger Liquids. There have also been applications to Kondo and Anderson lattices and ladders and models for manganites, the so-called Ferromagnetic Kondo Lattice model (see e.g. [24,25] for recent results).

There have been several improvements to the DMRG method like the inclusion of symmetries such as total spin, parity and momentum representation [26]. Other recent applications have been in nuclear shell model calculations where a two level pairing model has been considered[27] and in the study of ultrasmall superconducting grains, in this case, using the particle (hole) states around the Fermi level as the system (environment) block[28,29]. It has also been used in problems in high energy physics in toy models for QCD [30] and field theory models.

The DMRG has been very successfully extended to study classical systems. For a detailed description we refer the reader to Ref. [31]. Since 1D quantum systems are related to 2D classical systems[33], it is natural to adapt DMRG to the classical 2D case. This method is based on the renormalization group transformation for the transfer matrix T (TMRG)[32]. It is a variational method that maximizes the partition function using a limited number of degrees of freedom, where the variational state is written as a product of local matrices[17]. For 2D classical systems, this algorithm is superior to the classical Monte Carlo method in accuracy, speed and in the possibility of treating much larger systems. It was first applied to the Ising and Potts models and non-hermitian problems in equilibrium and non-equilibrium physics.

The application of the DMRG method to classical systems open the possibility to study 1D quantum systems at non zero temperature, by using the Trotter-Suzuki method [34,35,36,37,38] where the results are precise at high temperatures. In this case the system is infinite and the finiteness is in the level of the Trotter approximation. It has been applied to calculate thermodynamic properties for spin chains and ladders, Kondo insulator, Kondo impurities and t-J models.

A very promising extension of DMRG concerns molecules and its utilization in Quantum Chemistry. It has been used to calculate properties in long organic molecules, large Fe molecules, models for reptons and excitations in dendrimer molecules. Recent attempts to apply DMRG to the *ab initio* calculation of electronic states in molecules have been successful[39,40,41,42].

Another recent and important development concerns real-time calculations to study for example the evolution of wave functions or the calculation of transport properties in low-dimensional systems (the so-called time dependent DMRG). Early calculations based on the integration of the Schrödinger equation were performed in Ref. [43,44] and applied to the calculation of transport properties through a junction between two Luttinger liquids [45]. A very recent improvement based on the Trotter-Suzuki expansion of the evolution operator [46] was done by White and Feiguin [47], where they obtain vary accurate results and even obtain the frequency dynamics by Fourier transforming the real-time results.

4. DMRG for dynamical properties

DMRG can also be used to calculate dynamical properties of low-dimensional systems, useful to interpret experimental results from, for example, nuclear magnetic resonance (NMR), neutron scattering, optical absorption, photoemission, among others. There have been two main approaches to the dynamics, the Lanczos [48,49] and the correction vector techniques [50,51,49]. The first gives complete information of the whole excitation spectrum at the expense of less accuracy for large systems, specially at high energies. The latter, instead, focuses on particular energy values and give more precise information, but numerically much more expensive.

4.1. *Lanczos technique*

Suppose one wants to calculate the following dynamical correlation function at $T = 0$, $C_A(t-t') = \langle\psi_0|A^\dagger(t)A(t')|\psi_0\rangle$, where $A^\dagger$ is the Hermitean conjugate of the operator A, $A(t)$ is the Heisenberg representation of A, and $|\psi_0\rangle$ is the ground state of the system. Its Fourier transform is:

$$C_A(\omega) = \sum_n |\langle\psi_n|A|\psi_0\rangle|^2 \, \delta(\omega - (E_n - E_0)), \tag{1}$$

where the summation is taken over all the eigenstates $|\psi_n\rangle$ of the Hamiltonian H with energy E_n, and E_0 is the ground state energy.

Defining the Green's function $G_A(z) = \langle\psi_0|A^\dagger(z-H)^{-1}A|\psi_0\rangle$, the correlation function $C_A(\omega)$ can be obtained as

$$C_A(\omega) = -\frac{1}{\pi} \lim_{\eta\to 0^+} \mathrm{Im}\, G_A(\omega + i\eta + E_0). \tag{2}$$

The function G_A can be written in the form of a continued fraction:

$$G_A(z) = \cfrac{\langle\psi_0|A^\dagger A|\psi_0\rangle}{z - a_0 - \cfrac{b_1^2}{z - a_1 - \cfrac{b_2^2}{z - \cdots}}} \tag{3}$$

The coefficients a_n and b_n can be obtained using the following recursion equations [52,53]: $|f_{n+1}\rangle = H|f_n\rangle - a_n|f_n\rangle - b_n^2|f_{n-1}\rangle$, where $|f_0\rangle = A|\psi_0\rangle$, $a_n = \langle f_n|H|f_n\rangle/\langle f_n|f_n\rangle$ and $b_n^2 = \langle f_n|f_n\rangle/\langle f_{n-1}|f_{n-1}\rangle$, with $b_0 = 0$.

For finite systems the Green's function $G_A(z)$ has a finite number of poles so only a certain number of coefficients a_n and b_n have to be calculated. An important requirement is that the reduced Hilbert space should also describe with great precision the relevant excited states $|\psi_n\rangle$. This is achieved by choosing the appropriate target states. For most systems it is enough to consider as target states the ground state $|\psi_0\rangle$ and the first few $|f_n\rangle$ with $n = 0, 1...$ and $|f_0\rangle = A|\psi_0\rangle$ as described above. In doing so, states in the reduced Hilbert space relevant to the excited states connected to the ground state via the operator of interest A are included.

This method has been successfully applied to a number of problems, like spin 1/2 and 3/2 [48,54] and spin 1 chains[49], the spin-boson model [55], the Holstein model [56]

and spin-orbital chains in external fields [57]. It was also applied to extract spin-chain dispersion relations [58], dynamics of spin ladders [59], spectral functions in the infinite-U Hubbard model [60] and optical response in 1D Mott insulators [61]. In the Section 4 we will describe its application as the impurity solver within the Dynamical Mean Field Theory (DMFT) method.

4.2. *Correction vector dynamics*

This method focuses on a particular energy or energy window, allowing for a more precise description in that range and the possibility of calculating spectra for higher energies. Instead of using the tridiagonalization of the Hamiltonian, but in a similar spirit regarding the important target states to be kept, the spectrum can be calculated for a given $z = w + i\eta$ by using a correction vector (related to the operator A that can depend on momentum q).

Following the Green's function given above, the (complex) correction vector $|x(z)\rangle$ can be defined as:

$$|x(z)\rangle = \frac{1}{z - H} A|\psi_0\rangle \tag{4}$$

so the Green's function can be calculated as $G(z) = \langle\psi_0|A^\dagger|x(z)\rangle$.

Separating the correction vector in real and imaginary parts $|x(z)\rangle = |x^r(z)\rangle + i|x^i(z)\rangle$ we obtain

$$\begin{aligned} ((H - w)^2 + \eta^2)|x^i(z)\rangle &= -\eta A|\psi_0\rangle \\ |x^r(z)\rangle &= \frac{1}{\eta}(w - H)|x^i(z)\rangle \end{aligned} \tag{5}$$

The former equation is solved using the conjugate gradient method. In order to keep the information of the excitations at this particular energy the following states are targeted in the DMRG iterations: The ground state $|\psi_0\rangle$, the first Lanczos vector $A|\psi_0\rangle$ and the correction vector $|x(z)\rangle$. Even though only a certain energy is focused on, DMRG gives the correct excitations for an energy range surrounding this particular point so that by running several times for nearby frequencies, an approximate spectrum can be obtained for a wider region [49].

A variational formulation of the correction vector technique has been developed in [51]. It has been successfully applied to calculate the optical conductivity of Mott insulators.[62,63,64]

The correction vector model has also been applied to determine the nonlinear optical coefficients of Hubbard chains and related models [65], to calculate ac conductivity of the Bose-Hubbard model [66] and the single-impurity Anderson model.[67]

5. Dynamical Mean Field Theory using DMRG

The Dynamical Mean Field Theory (DMFT) has become one of the basic methods to calculate realistic electronic band structure in strongly correlated systems [68]. At

the heart of the DMFT method is the solution of an associated quantum impurity model where the environment of the impurity has to be determined self-consistently. Therefore the ability to obtain reliable DMFT solutions of lattice model Hamiltonians relies directly on the ability to solve quantum impurity models. Among the *a priori* exact numerical algorithms available we count the Hirsch-Fye Quantum Monte Carlo [69,70] method and Wilson's Numerical Renormalization Group (NRG) [71,72,73]. While the former, a finite-temperature method, is very stable and accurate at the Matsubara frequencies, its main drawback is the access to real frequency quantities for the calculation of spectral functions which requires less controlled techniques for the analytic continuation of the Green functions. The second method can be formulated both at T=0 and finite (small) T and provides extremely accurate results at very small frequencies, at the expense of a less accurate description of the high energy features.

In order to overcome the difficulties encountered by these other methods, we will show that DMRG can be used very reliably to solve the related impurity problem within DMFT[74]. By using the DMRG to solve the related impurity problem, no *a priori* approximations are made and the method provides equally reliable solutions for both gapless and gapfull phases. More significantly, it provides accurate estimates for the distributions of spectral intensities of high frequency features such as the Hubbard bands, that are of main relevance for analysis of x-ray photoemission and optical conductivity experiments.

We will now very briefly describe the method applied to the Mott thansition in the Hubbard model. The Hamiltonian of the Hubbard model is defined by

$$H = t \sum_{\langle i,j \rangle, \sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\downarrow} n_{i,\uparrow} \tag{6}$$

Applying DMFT to this model leads to a mapping of the original lattice model onto an associated quantum impurity problem in a self-consistent bath. In the particular case of the Hubbard model, the associated impurity problem is the single impurity Anderson model (SIAM), where the hybridization function $\Delta(\omega)$, which in the usual SIAM is a flat density of states of the conduction electrons, is now to be determined self-consistently. More precisely, for the Hamiltonian (6) defined on a Bethe lattice of coordination d, one takes the limit of large d and exactly maps the model onto a SIAM impurity problem with the requirement that $\Delta(\omega) = t^2 G(\omega)$, where $G(\omega)$ is the impurity Green's function. At the self-consistent point $G(\omega)$ coincides with the *local* Green's function of the original lattice model [75]. We take the half-bandwidth of the non interacting model as unit of energy, $t = 1/2$.

The Green's function of the impurity problem is an important quantity in this algorithm: $\mathrm{G}_0(\omega) = 1/(\omega + \mu - \Delta(\omega)) = 1/(\omega + \mu - t^2 G(\omega))$. Thus, to implement the new algorithm we shall consider [76,77] a general representation of the hybridization function in terms of continued fractions that define a *parametrization* of $\Delta(\omega)$ in terms of a set of real and positive coefficients. Since it is essentially a Green's function, $\Delta(z)$ can be decomposed into "particle" and "hole" con-

tributions as $\Delta(z) = \Delta^{>}(z) + \Delta^{<}(z)$ with $\Delta^{>}(z) = t^2\langle gs|c\frac{1}{z-(H-E_0)}c^{\dagger}|gs\rangle$ and $\Delta^{<}(z) = t^2\langle gs|c^{\dagger}\frac{1}{z+(H-E_0)}c|gs\rangle$ for a given Hamiltonian, H with ground-state energy E_0. By standard Lanczos technique, H can be in principle tri-diagonalized and the functions $\Delta^{>}(z)$ and $\Delta^{<}(z)$ can be expressed in terms of respective continued fractions[48]. As first implemented in Ref.[76,77], each continued fraction can be represented by a chain of auxiliary atomic sites whose energies and hopping amplitudes are given by the continued fraction diagonal and off-diagonal coefficients respectively.

As a result of the self-consistency condition, the two chains representing the hybridization, are "attached" to the right and left of an atomic site to obtain a new SIAM Hamiltonian, H. In fact $G_0(z)$ constitutes the local Green's function of the site plus chain system. The algorithm in Ref.[76,77], basically consists in switching on the local Coulomb interaction at the impurity site of the SIAM Hamiltonian and use the Lanczos technique to re-obtain $\Delta(z)$, iterating the procedure until the set of continued fractions coefficients converges. By using the DMRG, the number of auxiliary sites that can be used in the hybridization chains is much larger than in the exact diagonalization scheme, leading to more accurate results[78]. An alternative way of using DMRG to solve the impurity problem, which does not rely on the continued fraction expansion was developed in [79].

The SIAM Hamiltonian therefore reads

$$H = \sum_{\sigma,\alpha=-N_C;\alpha\neq 0}^{N_C} a_\alpha c^{\dagger}_{\alpha\sigma}c_{\alpha\sigma} + \sum_{\sigma,\alpha=-(N_C-1);\alpha\neq 0,-1}^{N_C-1} b_\alpha(c^{\dagger}_{\alpha\sigma}c_{\alpha+1\sigma} + h.c.) + \sum_{\sigma,\alpha=\pm 1} b_0(c^{\dagger}_{\sigma}c_{\alpha\sigma} + h.c.) + U(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2}) \quad (7)$$

with c_σ being the destruction operator at the impurity site, and $c_{\alpha\sigma}$ being the destruction operator at the α site of the hybridization chain of $2N_C$ sites. The set of parameters $\{a_\alpha, b_\alpha\}$ are directly obtained from the coefficients of the continued fraction representations of $\Delta(z)$ by the procedure just described.

In Fig.2 we show the DMFT+DMRG results (solid lines) for the density of states (DOS) for several values of increasing interaction U. The results are compared to the Iterated Perturbation Theory (IPT) results (dashed lines) [?,?].

Results for the imaginary part of the Green's funtions on the Matsubara frequencies match the precise Monte Carlo solutions at low temperatures. We also obtained accurate values for the two distinct critical values of the interaction $U_{c1} == 2.39 \pm 0.02$ and $U_{c2} = 3.0 \pm 0.2$. To this end, reaching larger system sizes turned out to be important in order to perform proper extrapolations and overcome finite-size effects.

6. Conclusions

In summary, the DMRG method has proven to be a very reliable and versatile numerical method that can be applied to a broad spectrum of problems in physics. In

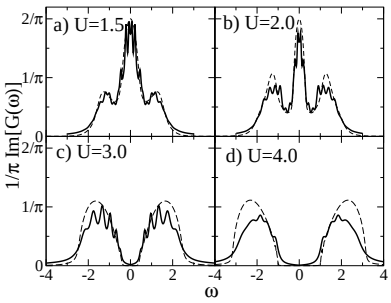

Fig. 2. Density of states ($\frac{1}{\pi}\mathrm{Im}G(\omega)$) for the half-filled Hubbard Model [?]. We also show the IPT results (dashed lines).

spite of having been developed twelve years ago, it's still evolving and it presents very interesting potential new applications. One of them was presented here for solving the DMFT equations of strongly correlated models exploiting the DMRG methodology. Large systems can be considered and accurate values of the critical interactions are obtained in agreement with NRG predictions allowing for a non-trivial test of the accuracy of this method. In contrast with NRG, however, this new algorithm deals with all energy scales on equal footing which allowed us to find interesting substructure in the Hubbard bands of the correlated metallic state. The ability of the new algorithm to directly deal with the high energy scales is a very important feature which is relevant for the interpretation of high resolution photoemission spectroscopies.[80] In addition, with this method, realistic band-structure calculations of systems with a larger number of degrees of freedom can be handled.

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