

CHAPTER 1

Numerical methods for nanoscopic systems based on density matrix renormalization

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1. Introduction

The Density Matrix Renormalization Group (DMRG) was developed by S. White in 1992 [1] and since then it 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. Since then 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 dimensional (2D) classical systems, stochastic models, the presence of 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. All these topics are treated in detail and in a pedagogical way in the book [2], where the reader can find an extensive review on DMRG and also in a recent review in [3].

In this chapter we will review the main aspects of the method. We also comment on some of the most relevant applications so as to give an overview on the scope and possibilities of DMRG and mention the most important extensions of the method.

When considering finite systems, the exponential growth of degrees of freedom to be considered imposes 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.

The DMRG was originally developed to overcome the problems that arise in interacting systems in 1D when standard RG procedures were applied. Consider a block B (a block is a collection of sites) where the Hamiltonian H_B and end-operators are defined. These traditional methods consist in putting together two or more blocks (e.g. B - B' , which we will call the superblock), connected using end-operators, in a basis that is a direct product of the basis of each block, forming $H_{BB'}$. This Hamiltonian is then diagonalized, the superblock is replaced by a new effective block B_{new} formed by a certain number m of lowest-lying eigenstates of $H_{BB'}$ and the iteration is continued (see Ref. [4]). Although it has been used successfully in certain cases, this procedure, or similar versions of it, has been applied to several interacting systems with poor performance. For example, it has been applied to the 1D Hubbard model keeping $m \simeq 1000$ states. For 16 sites, an error of 5-10% was obtained [5]. Other results [6] were also discouraging. A better performance was obtained [7] by adding a single site at a time rather than doubling the block size. However, there is one case where a similar version of this method applies very well: the Kondo (and Anderson) model. Wilson [8] mapped the one-impurity problem onto a one-dimensional lattice with exponentially decreasing hoppings. The difference with the method explained above is that in this case, one site (equivalent to an “onion shell”) is added at each step and, due to the exponential decrease of the hopping, very accurate results can be obtained.

Returning to the problem of putting several blocks together, the main source of error comes from the election of eigenstates of $H_{BB'}$ as representative states of a superblock. Since $H_{BB'}$ has no connection to the rest of the lattice, its eigenstates may have unwanted features (like nodes) at the ends of the block and this can't be improved by increasing the number of states kept. Based on this consideration, Noack and White [9] tried including different boundary conditions and boundary strengths. This turned out to work well for single particle and Anderson localization problems but, however, it did not improve the results significantly for interacting systems. These considerations led to the idea of taking a larger superblock that includes the blocks BB' , diagonalize the Hamiltonian in this large superblock and then somehow project the most favorable states onto BB' . Then BB' is replaced by B_{new} . In this way, awkward features in the boundary would vanish and a better representation of the states in the infinite system would be

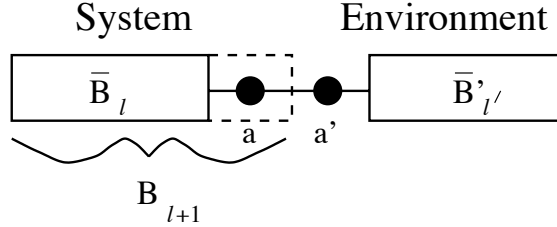


Fig. 1. A scheme of the superblock (universe) configuration for the DMRG algorithm [4].

achieved. White [1,4] proposed the density matrix as the optimal way of projecting the best states onto part of the system and this will be discussed in the next section. Some considerations concerning the effect of boundary conditions in the nature of the states kept (and an analogy to the physics of black holes) is given in [10]. The justification of using the density matrix is given in detail in Ref. [2]. A very easy and pedagogical way of understanding the basic functioning of DMRG is applying it to the calculation of simple quantum problems like one particle in a tight binding chain [11,12].

In the following Section we will briefly describe the standard method; in Sect. 3 we will mention some of the most important applications; in Sect. 4 we review the most relevant extensions to the method and finally; Sect. 5 will be devoted to the calculation of dynamical properties and, finally, in Sect. 6 we describe how DMRG can be used together with the Dynamical Mean Field Theory to obtain spectral properties of correlated systems.

2. The Method

The DMRG allows for a systematic truncation of the Hilbert space by keeping the most probable states describing a wave function (*e.g.* the ground state) instead of the lowest energy states usually kept in previous real space renormalization techniques.

The basic idea consists in starting with a small system (*e.g.* with N sites) and then gradually increase its size (to $N + 2$, $N + 4$,...) until the desired length is reached. Let us call the collection of N sites the *universe* and divide it into two parts: the *system* and the *environment* (see Fig. 1). The Hamiltonian is constructed in the *universe* and its ground state $|\psi_0\rangle$ is obtained. This is considered as the state of the *universe* and called the *target state*. It has components on the *system* and the *environment*. We want to obtain the most relevant states of the *system*, i.e., the states of the *system* that have largest weight in $|\psi_0\rangle$. To obtain this, the *environment* is considered as a statistical bath and the density matrix [13] is used to obtain the desired information on the *system*. So instead of keeping eigenstates of the Hamiltonian in the block (*system*), we keep eigenstates of the density matrix. We will be more explicit below.

Let's define block $[B]$ as a finite chain with l sites having an associated Hilbert space with m states where operators are defined (in particular the Hamiltonian in this finite chain, H_B and the operators at the ends of the block, useful for linking it to other chains or added sites). Except for the first iteration, the basis in this block isn't explicitly known due to previous basis rotations and reductions. The operators in this basis are matrices and the basis states are characterized by quantum numbers (like S^z , charge or number of particles, etc). We also define an added block or site as $[a]$ having n states. A general iteration of the method is described below:

i) Define the Hamiltonian $H_{BB'}$ for the superblock (the *universe*) formed by putting together two blocks $[B]$ and $[B']$ and two added sites $[a]$ and $[a']$ in this way: $[B \ a \ a' \ B']$ (the primes are only to indicate additional blocks, but the primed blocks have the same structure as the non-primed ones; this can vary, see the finite-size algorithm below). In general, blocks $[B]$ and $[B']$ come from the previous iteration. The total Hilbert space of this superblock is the direct product of the individual spaces corresponding to each block and the added sites. In practice a quantum number of the superblock can be fixed (in a spin chain for example one can look at the total $S^z = 0$ subspace), so the total number of states in the superblock is much smaller than $(mn)^2$. In some cases, as the quantum number of the superblock consists of the sum of the quantum numbers of the individual blocks, each block must contain several subspaces (several values of S^z for example). Here periodic boundary conditions can be attached to the ends and a different block layout should be considered (e.g. $[B \ a \ B' \ a']$) to avoid connecting blocks $[B]$ and $[B']$ which takes longer to converge. The boundary conditions are between $[a']$ and $[B]$. For closed chains the performance is poorer than for open boundary conditions [4, 14] (see Fig.2)

ii) Diagonalize the Hamiltonian $H_{BB'}$ to obtain the ground state $|\psi_0\rangle$ (target state) using Lanczos [15] or Davidson [16] algorithms. Other states could also be kept, such as the first excited ones: they are all called *target states*.

iii) Construct the density matrix:

$$\rho_{ii'} = \sum_j \psi_{0,ij} \psi_{0,i'j} \quad (1)$$

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 $[B' \ a']$, as a statistical bath. The eigenstates of ρ with the highest eigenvalues correspond to the most probable states (or equivalently the states with highest weight) of block $[B \ a]$ in the ground state of the whole superblock. These states are kept up to a certain cutoff, keeping a total of m states per block. The density matrix eigenvalues, ω_α , sum up to unity and the truncation error, defined as the sum of the density matrix eigenvalues corresponding to discarded eigenvectors, $\sum_{\alpha=m+1}^{m_{max}} \omega_\alpha$, gives a qualitative indication of the accuracy of the calculation.

iv) With these m states a rectangular matrix O is formed and it is used to change basis and reduce all operators defined in $[B \ a]$. This block $[B \ a]$ is then renamed as block $[B_{new}]$ or simply $[B]$ (for example, the Hamiltonian in block $[B \ a]$, H_{Ba} , is transformed into H_B as $H_B = O^\dagger H_{Ba} O$).

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

vi) This iteration continues until the desired length is achieved. At each step the length is $N = 2l + 2$ (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:

$$\rho_{ii'} = \sum_l p_l \sum_j \phi_{l,ij} \phi_{l,i'j} \quad (2)$$

where p_l defines the probability of finding the system in the target state $|\phi_l\rangle$ (not necessarily 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 (see Fig. 2). In order to keep N fixed, in the next block configuration, the right block B' should be

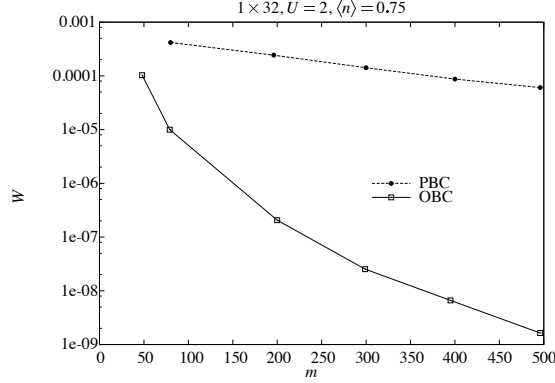


Fig. 2. Truncation error for the finite-system DMRG as a function of the number of states kept m (from [11], with permission).

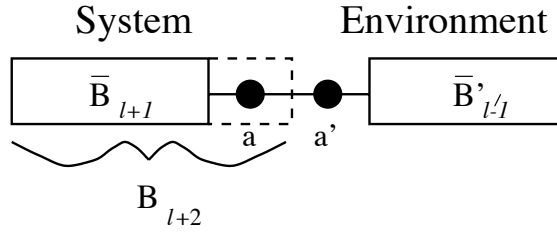


Fig. 3. One step of the finite-size algorithm, where the total length $N = 2l + 2$ is fixed.

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 $N - 2$) [2]. With this method, a higher precision can be achieved (see Fig. ??).

As an example of a general DMRG building step let's look at the one-dimensional Heisenberg model

$$H = \sum_i \mathbf{S}_i \mathbf{S}_{i+1} = S_i^z S_{i+1}^z + \frac{1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+). \quad (3)$$

Suppose we want to connect two blocks $[B_1 = \mathbf{B} \mathbf{a}]$, defined by states i, j , with $[B_2 = \mathbf{a}' \mathbf{B}']$, defined by states i', j' , to form the Hamiltonian in the superblock, which we will diagonalize to get the energies and eigenstates. Performing an external product between the operators we have stored from previous iterations we have:

$$\begin{aligned} [H_{B_1 B_2}]_{ij; i' j'} &= [H_{B_1}]_{ii'} \delta_{jj'} + [H_{B_2}]_{jj'} \delta_{ii'} + [S_a^z]_{ii'} [S_{a'}^z]_{jj'} \\ &\quad + \frac{1}{2} [S_a^+]_{ii'} [S_{a'}^-]_{jj'} + \frac{1}{2} [S_a^-]_{ii'} [S_{a'}^+]_{jj'} \end{aligned} \quad (4)$$

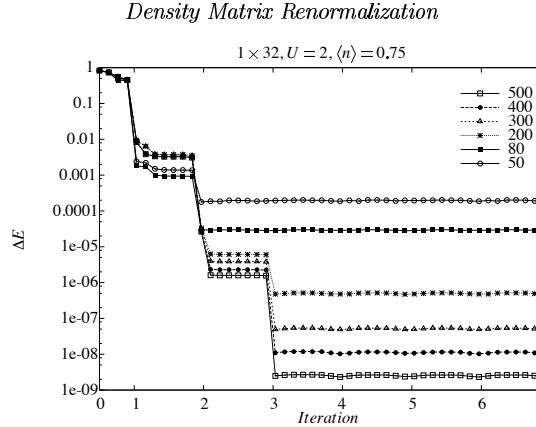


Fig. 4. Difference between the ground-state energy obtained from the *finite system* DMRG with different number of iterations and number of states kept m , and the exact energy calculated using Bethe Ansatz for a 32-site Hubbard model ($U = 2$ and filling $n = 3/4$). Reprinted from [11] with permission.

If fermionic models are to be considered, more operators are to be kept, such as, for example, the creation and destruction operators at the borders of the blocks to perform the interblock hopping.

The calculation of static properties like correlation functions is easily done by keeping the operators at each step and performing the corresponding basis change and reduction, in a similar manner as done with the Hamiltonian in each block [4]. The energy and measurements are calculated in the superblock. In Ref. [17] 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 [18,19] has focused on the quantum information perspective of DMRG by calculating the von Neumann entropy of entanglement in a block:

$$S = -\text{Tr} \hat{\rho} \ln_2 \hat{\rho} = -\sum_{\alpha} \omega_{\alpha} \ln_2 \omega_{\alpha} \quad (5)$$

In performing the DMRG truncation, maximum entanglement between system and environment is achieved.

Within this frame it can be shown that DMRG, in its present form, is not suited for calculations in dimensions higher than one. Although calculations in 2D have been performed, the DMRG does not have the potentiality it has for 1D systems. In Fig. 5 we show a general sweeping scheme for the 2D case (for applications see below).

A faster convergence of Lanczos or Davidson algorithm is achieved by choosing a good trial vector [20,21]. An interesting analysis on DMRG accuracy is done in Ref. [22]. Fixed points of the DMRG and their relation to matrix product wave functions were studied in [23] and an analytic formulation combining the block renormalization group with variational and Fokker-Planck methods in [24]. The connection of the method with quantum groups and conformal field theory is treated in [25]. There are also interesting connections between the density matrix spectra and integrable models [26] via corner transfer matrices. These articles give a deep insight into the essence of the DMRG method.

3. Applications

Since its development, the number of papers using DMRG has grown enormously and other improvements to the method have been performed. For example, since 1998 there have been around 80 papers a year using DMRG. There have also been several improvements to the method and it is now used in areas

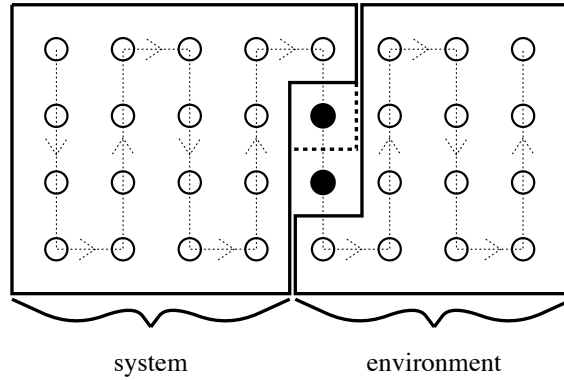


Fig. 5. General sweeping and superblock configuration for a two-dimensional lattice (from [11], with permission)

that are very different to the original strongly correlated electron system field. We would like to mention some applications where this method has proved to be useful. Other applications related to further developments of the DMRG will be mentioned in Sect. 4.

A very impressive result with unprecedented accuracy was obtained by White and Huse [27] when calculating the spin gap in a $S = 1$ Heisenberg chain obtaining $\Delta = 0.41050J$. They also calculated very accurate spin correlation functions and excitation energies for one and several magnon states and performed a very detailed analysis of the excitations for different momenta. They obtained a spin correlation length of 6.03 lattice spacings. Simultaneously Sørensen and Affleck [28] also calculated the structure factor and spin gap for this system up to length 100 with very high accuracy, comparing their results with the nonlinear σ model. In a subsequent paper [29] they applied the DMRG to the anisotropic $S = 1$ chain, obtaining the values for the Haldane gap. They also performed a detailed study of the $S = 1/2$ end excitations in an open chain. Thermodynamical properties in open $S = 1$ chains such as specific heat, electron paramagnetic resonance (EPR) and magnetic susceptibility calculated using DMRG gave an excellent fit to experimental data, confirming the existence of free spins $1/2$ at the boundaries [30]. A related problem, *i.e.* the effect of non-magnetic impurities in spin systems (dimerized, ladders and 2D) was studied in [31,32]. In addition, the study of magnon interactions and magnetization of $S = 1$ chains was done in [33], supersymmetric spin chains modelling plateau transitions in the integer quantum Hall effect in [34] and ESR studies in these systems was considered in [35]. For larger integer spins there have also been some studies. Nishiyama and coworkers [36] calculated the low energy spectrum and correlation functions of the $S = 2$ antiferromagnetic Heisenberg open chain. They found $S = 1$ end excitations (in agreement with the Valence Bond Theory). Edge excitations for other values of S have been studied in Ref. [37]. Almost at the same time Schollwöck and Jolicoeur [38] calculated the spin gap in the same system, up to 350 sites, ($\Delta = 0.085J$), correlation functions that showed topological order and a spin correlation length of 49 lattice spacings. More recent accurate studies of $S = 2$ chains are found in [39–41] and of $S = 1$ chains in staggered magnetic fields [42] including a detailed comparison to the non-linear sigma model in [43]. In Ref. [44] the dispersion of the single magnon band and other properties of the $S = 2$ antiferromagnetic Heisenberg chains were calculated.

Concerning $S = 1/2$ systems, DMRG has been crucial for obtaining the logarithmic corrections to the $1/r$ dependence of the spin-spin correlation functions in the isotropic Heisenberg model [45]. For this, very accurate values for the energy and correlation functions were needed. For $N = 100$ sites

an error of 10^{-5} was achieved keeping $m = 150$ states per block, comparing with the exact finite-size Bethe Ansatz results. For this model it was found that the data for the correlation function has a very accurate scaling behaviour and advantage of this was taken to obtain the logarithmic corrections in the thermodynamic limit. Other calculations of the spin correlations have been performed for the isotropic [46, 47] and anisotropic cases [48]. Luttinger liquid behaviour with magnetic fields have been studied in [49], field-induced gaps and string order parameters in [50] and [51] respectively, anisotropic systems in [52, 53] and the Heisenberg model with a weak link in [54]. An analysis of quantum critical points and critical behaviour in spin chains by combining DMRG with finite-size scaling was done in [55].

Similar calculations have been performed for the $S = 3/2$ Heisenberg chain [56]. In this case a stronger logarithmic correction to the spin correlation function was found. For this model there was interest in obtaining the central charge c to elucidate whether this model corresponds to the same universality class as the $S = 1/2$ case, where the central charge can be obtained from the finite-size scaling of the energy. Although there have been previous attempts [57], these calculations presented difficulties since they involved also a term $\sim 1/\ln^3 N$. With the DMRG the value $c = 1$ was clearly obtained.

In Ref. [58], DMRG was applied to an effective spin Hamiltonian obtained from an $SU(4)$ spin-orbit critical state in 1D. Other applications were done to enlarged symmetry cases with $SU(4)$ symmetry in order to study coherence in arrays of quantum dots [59], to obtain the phase diagram for 1D spin orbital models [60] and dynamical properties in a magnetic field [61].

Dimerization and frustration have been considered in Refs. [62–70] and alternating spin chains in [71].

The case of several coupled spin chains (ladder models) have been investigated in [72–76], spin ladders with cyclic four-spin exchanges in [77, 78, 80, 264] and Kagome antiferromagnets in [81]. Zigzag spin chains have been considered in [82–84] and spin chains of coupled triangles in [85–87]. As the DMRG's performance is optimal in open systems, an interesting analysis of the boundary effect on correlation functions is done in [14]. Magnetization properties and plateaus for quantum spin ladder systems [88–90] have also been studied. An interesting review on the applications to some exact and analytical techniques for quantum magnetism in low dimension, including DMRG, is presented in [91].

There has been a great amount of applications to fermionic systems such as 1D Hubbard and t-J models [92, 94–102, 265], Luttinger liquids with boundaries [103], the Falicov-Kimball model [104], the quasiperiodic Aubry-Andre chain [105] and Fibonacci-Hubbard models [106]. It has also been applied to field theory [10, 107]. The method has been very successful for several band Hubbard models [108], Hubbard ladders [109–111] and t-J ladders [112]. Also several coupled chains at different dopings have been considered [113, 114] as well as flux phases in these systems [115]. Time reversal symmetry-broken fermionic ladders have been studied in [116] and power laws in spinless-fermion ladders in [117]. Long-range Coulomb interactions in the 1D electron gas and the formation of a Wigner crystal was studied in [118]. Several phases including the Wigner crystal, incompressible and compressible liquid states, stripe and pairing phases, have been found using DMRG for 2D electrons in high magnetic fields considering different Landau levels [119]. Persistent currents in mesoscopic systems have been considered in [120].

Quite large quasi-2D systems can be reached, for example in [121] where a 4×20 lattice was considered to study ferromagnetism in the infinite-U Hubbard model; the ground state of a 4-leg t-J ladder in [122]; the one and two hole ground state in 9×9 and 10×7 t-J lattices in [123]; a doped 3-leg t-J ladder in [124]; the study of striped phases in [125]; domain walls in 19×8 t-J systems in [126]; the 2D t-J model in [127] and the magnetic polaron in a 9×9 t-J lattice in [128]. Also big CaV_4O_9 spin-1/2 lattices reaching 24×11 sites [20] have been studied. There have been some recent attempts to implement DMRG in two and higher dimensions [129–133] but the performance is still poorer than in 1D. A recent extension using a two-step DMRG algorithm for highly anisotropic spin systems has shown promising results [134].

Impurity problems have been studied for example in one- [135] and two-impurity [136] Kondo systems, in spin chains [137] and in Luttinger Liquids [138]. There have also been applications to Kondo

and Anderson lattices [139–148], Kondo lattices with localized f^2 configurations [149], the two-channel Kondo lattice on a ladder [150], a t-J chain coupled to localized Kondo spins [151] and ferromagnetic Kondo models for manganites [152–154]. See also Refs. [155, 156] for recent results for the antiferro and ferromagnetic Kondo lattice models.

4. Other extensions to DMRG

There have been several extensions to DMRG like the inclusion of symmetries to the method such as spin and parity [158, 159, 254]. Total spin conservation and continuous symmetries have been treated in [147] and in interaction-round a face Hamiltonians [160], a formulation that can be applied to rotational-invariant systems like $S = 1$ and 2 chains [40]. A momentum representation of this technique [114, 130, 161] that allows for a diagonalization in a fixed momentum subspace has been developed as well as applications in dimension higher than one [20, 129, 130, 162] and Bethe lattices [163]. The inclusion of symmetries is essential to the method since it allows to consider a smaller number of states, enhance precision and obtain eigenstates with definite quantum numbers. Other recent applications have been in nuclear shell model calculations where a two level pairing model has been considered [164] 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 [165]. For a review on these applications see the recent publication [166].

A very interesting and successful application is a recent work in High Energy Physics [167]. Here the DMRG is used in an asymptotically free model with bound states, a toy model for quantum chromodynamics, namely the two dimensional delta-function potential. For this case an algorithm similar to the momentum space DMRG [161] was used where the block and environment consist of low and high energy states respectively. The results obtained here are much more accurate than with the similarity renormalization group [168] and a generalization to field-theoretical models is proposed based on the discrete light-cone quantization in momentum space [169]. Below we briefly mention other important extensions, leaving the calculation of dynamical properties for the next Section.

4.1. Classical systems

The DMRG has been very successfully extended to study classical systems. For a detailed description we refer the reader to Ref. [170]. Since 1D quantum systems are related to 2D classical systems [171], 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) [172]. 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 [23]. 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. A recent improvement of this method considering periodic boundary conditions is given in [173] and a detailed comparison between symmetric and asymmetric targetting is done in [174]. TMRG has also been successfully used to renormalize stochastic transfer matrices in a study of cellular automata [175]. The calculation of thermodynamical properties of 3D classical statistical systems has been proposed [131] where the eigenstate of the transfer matrix with maximum eigenvalue is represented by the product of local tensors optimized using DMRG.

A further improvement to this method is based on the corner transfer matrix [176], the CTMRG [178–180, 263] and can be generalized to any dimension [181].

It was first applied to the Ising model [170, 182–184] and also to the Potts model [185], where very accurate density profiles and critical indices were calculated. Further applications have included non-hermitian problems in equilibrium and non-equilibrium physics. In the first case, transfer matrices may be non-hermitian and several situations have been considered: a model for the Quantum Hall effect [186], the

q -symmetric Heisenberg chain related to the conformal series of critical models [187] and the anisotropic triangular nearest and next-nearest neighbour Ising models [87]. In the second case, the adaptation of the DMRG to non-equilibrium physics like the asymmetric exclusion problem [188] and reaction-diffusion problems [189,190] has shown to be very successful. It has also been applied to stochastic lattice models like in [191] and to the 2D XY model [192].

4.2. *Finite-temperature DMRG*

The adaptation of the DMRG method for classical systems paved the way for the study of 1D quantum systems at non zero temperature, by using the Trotter-Suzuki method [193–197] (see also a recent review in Ref. [198]). In this case the system is infinite and the finiteness is in the level of the Trotter approximation. Standard DMRG usually produces its best results for the ground state energy and less accurate results for higher excitations. A different situation occurs here: the lower the temperature, the less accurate the results.

Very nice results have been obtained for the dimerized, $S = 1/2$, XY model, where the specific heat was calculated involving an extremely small basis set [193] ($m = 16$), the agreement with the exact solution being much better in the case where the system has a substantial gap. It has also been used to calculate thermodynamical properties of the anisotropic $S = 1/2$ Heisenberg model, with relative errors for the spin susceptibility of less than 10^{-3} down to temperatures of the order of $0.01J$ keeping $m = 80$ states [195]. A complete study of thermodynamical properties like magnetization, susceptibility, specific heat and temperature dependent correlation functions for the $S = 1/2$ and $3/2$ Heisenberg models was done in [199]. Other applications have been the calculation of the temperature dependence of the charge and spin gap in the Kondo insulator [200], the calculation of thermodynamical properties of ferrimagnetic chains [3] and spin ladders [90], the study of impurity properties in spin chains [202,203], frustrated quantum spin chains [201], t-J [205] and spin ladders [206] and dimerized frustrated Heisenberg chains [207].

An alternative way of incorporating temperature into the DMRG procedure was developed by Moukouri and Caron [208]. They considered the standard DMRG taking into account several low-lying target states (see Eq. 2) to construct the density matrix, weighted with the Boltzmann factor (β is the inverse temperature):

$$\rho_{ii'} = \sum_l e^{-\beta E_l} \sum_j \phi_{l,ij} \phi_{l,i'j} \quad (6)$$

With this method they performed reliable calculations of the magnetic susceptibility of quantum spin chains with $S = 1/2$ and $3/2$, showing excellent agreement with Bethe Ansatz exact results. They also calculated low temperature thermodynamical properties of the 1D Kondo Lattice Model [209] and of organic conductors [210]. Zhang et al. [261] applied the same method in the study of a magnetic impurity embedded in a quantum spin chain.

4.3. *Phonons, bosons and disorder*

A significant limitation to the DMRG method is that it requires a finite basis and calculations in problems with infinite degrees of freedom per site require a large truncation of the basis states [212]. However, Jeckelmann and White developed a way of including phonons in DMRG calculations by transforming each boson site into several artificial interacting two-state pseudo-sites and then applying DMRG to this interacting system [213] (called the “pseudo-site system”). The idea is based on the fact that DMRG is much better able to handle several few-states sites than few many-state sites [214]. The key idea is to substitute each boson site with 2^N states into N pseudo-sites with 2 states [215]. They applied this method

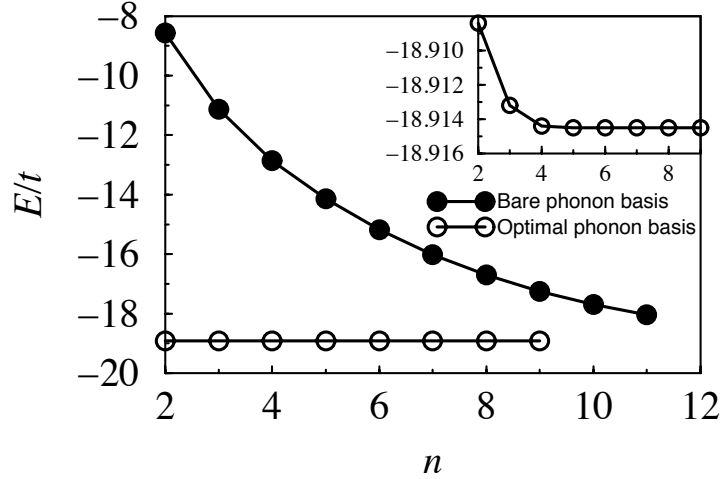


Fig. 6. Ground-state energy of a 4 site, half-filled Holstein system as a number of phonon states kept on each site of the lattice, for the optimal and bare phonon basis. Reprinted from [216] with permission.

to the Holstein model for several hundred sites (keeping more than a hundred states per phonon mode) obtaining negligible error. In addition, up to date, this method is the most accurate one to determine the ground state energy of the polaron problem (Holstein model with a single electron).

An alternative method (the “Optimal phonon basis”) [216] is a procedure for generating a controlled truncation of a large Hilbert space, which allows the use of a very small optimal basis without significant loss of accuracy. The system here consists of only one site and the environment has several sites, both having electronic and phononic degrees of freedom. The density matrix is used to trace out the degrees of freedom of the environment and extract the most relevant states of the site in question. In following steps, more bare phonons are included to the optimal basis obtained in this way. This method was successfully applied to study the Holstein model (Fig.6, the interactions induced by quantum fluctuations in quantum strings, as an application to cuprate stripes [217] and the dissipative two-state system [218]. A variant of this scheme is the “four block method”, as described in [219]. They obtain very accurately the Luttinger liquid-CDW insulator transition in the 1D Holstein model for spinless fermions.

The method has also been applied to pure bosonic systems such as the disordered bosonic Hubbard model [220], where gaps, correlation functions and superfluid density are obtained. The phase diagram for the non-disordered Bose-Hubbard model, showing a reentrance of the superfluid phase into the insulating phase was calculated in Ref. [221]. It has also been used to study a chain of oscillators with optical phonon spectrum [222] and optical phonons in the quarter-filled Hubbard model for organic conductors [223].

The DMRG has also been generalized to 1D random and disordered systems, and applied to the random antiferromagnetic and ferromagnetic Heisenberg chains [224], including quasiperiodic exchange modulation [225] and a detailed study of the Haldane [226] and Griffiths phase [227] in these systems. Strongly disordered spin ladders have been considered in [228]. It has also been used in disordered Fermi systems such as the spinless model [229,230]. In particular, the transition from the Fermi glass to the Mott insulator and the strong enhancement of persistent currents in the transition was studied in correlated one-dimensional disordered rings [231]. Disorder-induced crossover effects at quantum critical points were studied in [232].

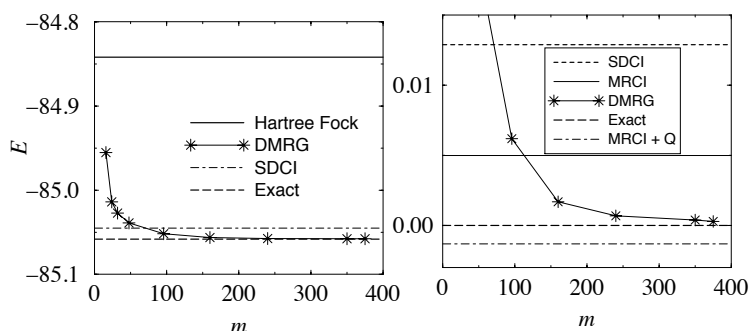


Fig. 7. Ground state energy (left) and error (right) of a water molecule in a 25 orbital basis using several methods. The DMRG results are plotted as a function of the number of states kept, m (not relevant for the other energies). Reprinted from [240] with permission.

4.4. Molecules and Quantum Chemistry

There have been several applications to molecules and polymers, such as the Pariser-Parr-Pople (PPP) Hamiltonian for a cyclic polyene [233] (where long-range interactions are included), magnetic Keplerate molecules [234], molecular Iron rings [235] and polyacenes considering long range interactions [236]. It has also been applied to conjugated organic systems (polymers), adapting the DMRG to take into account the most important symmetries in order to obtain the desired excited states [254]. Also conjugated one-dimensional semiconductors [237] have been studied, in which the standard approach can be extended to complex 1D oligomers where the fundamental repeat is not just one or two atoms, but a complex molecular building block. Relatively new fields of application are the calculation of dynamical properties in the Rubinstein-Duke model for reptons [238] and excitons in dendrimer molecules [239].

Recent attempts to apply DMRG to the *ab initio* calculation of electronic states in molecules have been successful [240–243]. Here, DMRG is applied within the conventional quantum chemical framework of a finite basis set with non-orthogonal basis functions centered on each atom. After the standard Hartree-Fock (HF) calculation in which a Hamiltonian is produced within the orthogonal HF basis, DMRG is used to include correlations beyond HF, where each orbital is treated as a “site” in a 1D lattice. One important difference with standard DMRG is that, as the interactions are long-ranged, several operators must be kept, making the calculation somewhat cumbersome. However, very accurate results have been obtained in a check performed in a water molecule (keeping up to 25 orbitals and $m \simeq 200$ states per block), obtaining an offset of 0.00024 Hartrees with respect to the exact ground state energy [244], a better performance than any other approximate method [240] (see Fig.7).

In order to avoid the non-locality introduced in the treatment explained above, White introduced the concept of *orthlets*, local, orthogonal and compact wave functions that allow prior knowledge about singularities to be incorporated into the basis and an adequate resolution for the cores [241]. The most relevant functions in this basis are chosen via the density matrix. An application based on the combination with the momentum version of DMRG is used in [245] to calculate the ground state of several molecules.

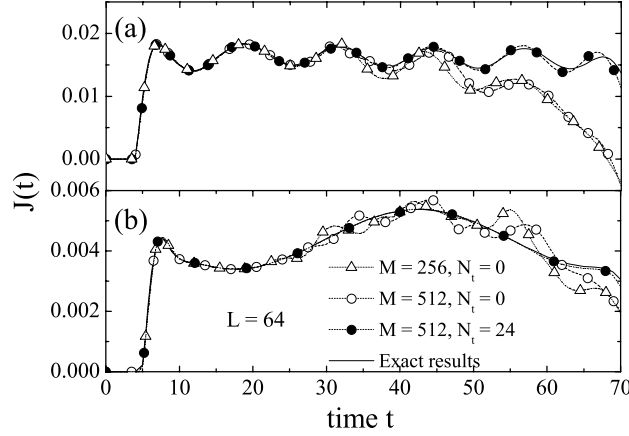


Fig. 8. Current through a) a non-interacting quantum dot and b) a junction between two leads (defined in [246]). N_t is the number of excited target states (reprinted with permission from [248]).

4.5. Time-dependent DMRG

Another recent and important development concerns real-time calculations: the so-called time dependent DMRG. Its potential applications include the analysis of the evolution of wave functions, the calculation of transport properties in low-dimensional systems, non-equilibrium transport through nanosystems or dissipative quantum mechanics.

There are two main different schemes to tackle time-dependent problems. Both different approaches have been classified as *static* and *dynamic* or *adaptive* time-dependent methods. In the first case the Hilbert space for the initial wave function is kept as large as possible so as to be able to describe the time-evolved state for sufficiently long times. In the second approach, instead, the states kept are calculated at each time interval, adapting to the evolving Hamiltonian.

The *static* method was developed by Cazalilla and Marston [246]. After growing the system up to a certain size, a quantum dot or a junction is added and a time-dependent perturbation is $H'(t)$ set on. The time-dependent Schrödinger equation is then integrated forward in time using a discretized algorithm:

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = [(H_{\text{trunc}} - E_0) + H'(t)] |\Psi(t)\rangle. \quad (7)$$

where the initial state is chosen to be the ground state of the unperturbed system. If more than one target state is used during the growing procedure (this means that the perturbation has to be added from the beginning), a higher precision is obtained and the time evolution can be followed longer [248]. Fig. 8 shows the current through two quantum systems calculated using this method.

A slightly different approach was used by Schmitteckert [247]. Instead of using the differential equation, he applied the time evolution operator $\exp(-iHt)$ directly by using a Krylov basis expansion of the matrix exponential. He calculates transport properties through small interacting nanostructures.

The *dynamic* or *adaptive* approach [249, 250] was based on the algorithm developed by Vidal for the time evolution of weakly entangled quantum states [251], originally formulated in the matrix product language.

The time evolution operator $\exp(-iH\tau)$ can be decomposed using a Trotter-Suzuki expansion into link operators (to order τ^3) as:

$$e^{-i\tau H} \approx e^{-i\tau H_1/2} e^{-i\tau H_2/2} \dots e^{-i\tau H_2/2} e^{-i\tau H_1/2}, \quad (8)$$

where H_i is the Hamiltonian term acting on lin i .

When applied $1/\tau$ times to get one time interval, the error is of the order τ^2 . One important characteristic of the DMRG is that, when operators are calculated acting on the single sites outside the renormalized blocks, the result is exact. Taking advantage of this, the above decomposition can be applied sequentially on these exact sites, in a finite-sweep like procedure. This algorithm can be easily incorporated into a static DMRG code. Using this method, White and Feiguin calculated the same transport properties as in Fig. 8 and their results match the exact result (full line) very precisely. They also calculated other time-dependent responses like the dispersion of a spin excitation in a 200-sites spin-1 Heisenberg chain (see Fig. 9).

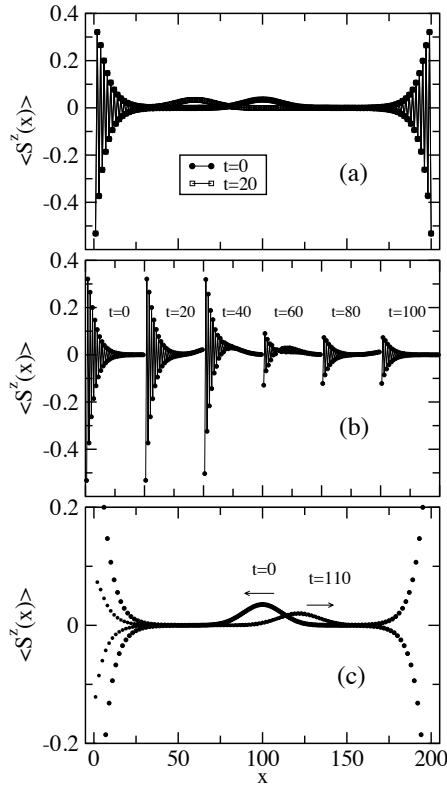


Fig. 9. Time evolution of a spin excitation wave-packet in a spin-1 Heisenberg 200-sites chain. In b) only the 50 leftmost sites are shown. Reprinted from [249] with permission.

The results obtained by this method are very accurate thus allowing to obtain frequency-dependent quantities by Fourier transformation [249].

5. Dynamical correlation functions

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 [252, 253] and the correction vector techniques [253–255]. 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.

An interesting development for calculating response functions in single impurity systems in the presence of a magnetic field was done in [256] by using the DMRG within Wilson's NRG to obtain the Green's function.

5.1. Lanczos technique

We want to calculate the following dynamical correlation function at $T = 0$:

$$C_A(t - t') = \langle \psi_0 | A^\dagger(t) A(t') | \psi_0 \rangle, \quad (9)$$

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:

$$C_A(\omega) = \sum_n |\langle \psi_n | A | \psi_0 \rangle|^2 \delta(\omega - (E_n - E_0)), \quad (10)$$

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

$$G_A(z) = \langle \psi_0 | A^\dagger (z - H)^{-1} A | \psi_0 \rangle, \quad (11)$$

the correlation function $C_A(\omega)$ can be obtained as

$$C_A(\omega) = -\frac{1}{\pi} \lim_{\eta \rightarrow 0^+} \text{Im} G_A(\omega + i\eta + E_0). \quad (12)$$

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

$$G_A(z) = \frac{\langle \psi_0 | A^\dagger A | \psi_0 \rangle}{z - a_0 - \frac{b_1^2}{z - a_1 - \frac{b_2^2}{z - \dots}}} \quad (13)$$

The coefficients a_n and b_n can be obtained using the following recursion equations [257, 258]:

$$|f_{n+1}\rangle = H|f_n\rangle - a_n|f_n\rangle - b_n^2|f_{n-1}\rangle \quad (14)$$

where

$$\begin{aligned} |f_0\rangle &= A|\psi_0\rangle \\ a_n &= \langle f_n | H | f_n \rangle / \langle f_n | f_n \rangle, \\ b_n^2 &= \langle f_n | f_n \rangle / \langle f_{n-1} | f_{n-1} \rangle; \quad b_0 = 0 \end{aligned} \quad (15)$$

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. The DMRG technique presents a good framework to calculate such quantities. With it, the ground state, Hamiltonian and the operator A required for the evaluation of $C_A(\omega)$ are obtained. An important requirement is that the reduced Hilbert space should also describe

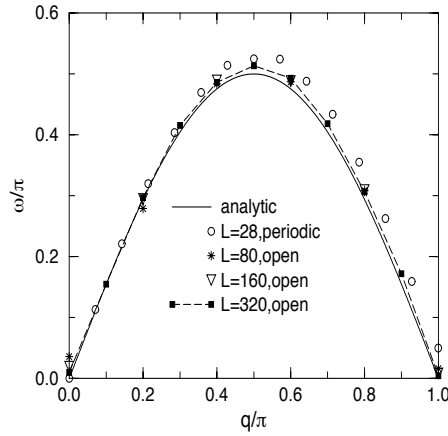


Fig. 10. Lower bound of the continuous excitation band of the AF $S = 1/2$ Heisenberg model for different system sizes L (reprinted from Ref. [253] with permission). The full line is the analytical result for the infinite system using Bethe Ansatz.

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 $n = 0, 1, \dots$ 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. The fact that $|f_0\rangle$ is an excellent trial state, in particular, for the lowest triplet excitations of the two-dimensional antiferromagnet was shown in Ref. [259]. Of course, if the number m of states kept per block is fixed, the more target states considered, the less precisely each one of them is described. An optimal number of target states and m have to be found for each case. Due to this reduction, the algorithm can be applied up to certain lengths, depending on the states involved. For longer chains, the higher energy excitations will become inaccurate. Proper sum rules have to be calculated to determine the errors in each case.

This method has been successfully applied to a number of problems, like spin $1/2$ (see Fig.10) and $3/2$ [45, 56, 252, 253] and spin 1 chains [253], the spin-boson model [260], the Holstein model [261] and spin-orbital chains in external fields [262]. It was also applied to extract spin-chain dispersion relations [263], dynamics of spin ladders [264], spectral functions in the infinite-U Hubbard model [265] and optical response in 1D Mott insulators [266]. In Section 4 we will describe its application as the impurity solver within the Dynamical Mean Field Theory method (DMFT).

5.2. 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:

$$|x(z)\rangle = \frac{1}{z - H} A |\psi_0\rangle \quad (16)$$

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

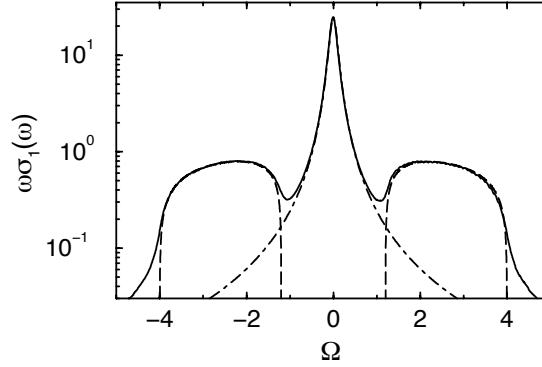


Fig. 11. Reduced optical conductivity for the Hubbard-Peierls model in the large- U limit and 128 sites (solid line). Here $\Omega = \omega - U$. For a comparison, a broadened delta peak at $\omega = U$ (dot-dashed) and thermodynamic results (dashed) are shown (reprinted from Ref. [255] with permission).

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

$$\begin{aligned} ((H - w)^2 + \eta^2)|x^i(z)\rangle &= -\eta A|\psi_0\rangle \\ |x^r(z)\rangle &= \frac{1}{\eta}(w - H)|x^i(z)\rangle \end{aligned} \quad (17)$$

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 [253].

A variational formulation of the correction vector technique has been developed in [255]. It has been successfully applied to calculate the optical conductivity of Mott insulators [267–269] (see, for example, Fig. 11).

The correction vector model has also been applied to determine the nonlinear optical coefficients of Hubbard chains and related models [270], to calculate ac conductivity of the Bose-Hubbard model [271] and the single-impurity Anderson model. [272]

5.3. Finite temperature dynamics

In order to include temperature in the calculation of dynamical quantities, the Transfer Matrix RG described above (TMRG [193, 195, 197]) was extended to obtain imaginary time correlation functions [273–275]. After Fourier transformation in the imaginary time axis, analytic continuation from imaginary to real frequencies is done using maximum entropy (ME). The combination of the TMRG and ME is free from statistical errors and the negative sign problem of Monte Carlo methods. Since we are dealing with the transfer matrix, the thermodynamic limit can be discussed directly without extrapolations. However, in the present scheme, only local quantities can be calculated.

A systematic investigation of local spectral functions is done in Ref. [275] for the anisotropic Heisenberg antiferromagnetic chain. The authors obtain good qualitative results especially for high temperatures but a quantitative description of peaks and gaps are beyond the method, due to the severe intrinsic limitation of the analytic continuation. This method was also applied with great success to the 1D Kondo

insulator [274]. The temperature dependence of the local density of states and local dynamic spin and charge correlation functions were calculated.

6. 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 [276]. 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 [277,278] method and Wilson's Numerical Renormalization Group (NRG) [279–281]. 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 [282]. 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 transition in the Hubbard model. The Hamiltonian of the Hubbard model is defined by

$$H = t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\downarrow} n_{i,\uparrow} \quad (18)$$

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 (18) 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 [283]. 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: $G_0(\omega) = 1/(\omega + \mu - \Delta(\omega)) = 1/(\omega + \mu - t^2 G(\omega))$. Thus, to implement the new algorithm we shall consider [284,285] 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” contributions 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 [252]. As first implemented in Ref. [284,285], 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. [284,285], 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 [286]. An alternative way of using DMRG to solve the impurity problem, which does not rely on the continued fraction expansion was developed in [287].

The SIAM Hamiltonian therefore reads

$$H = \sum_{\sigma, \alpha=-N_C; \alpha \neq 0}^{N_C} a_{\alpha} c_{\alpha\sigma}^{\dagger} c_{\alpha\sigma} + \sum_{\sigma, \alpha=-(N_C-1); \alpha \neq 0, -1}^{N_C-1} b_{\alpha} (c_{\alpha\sigma}^{\dagger} c_{\alpha+1\sigma} + h.c.) + \sum_{\sigma, \alpha=\pm 1} b_0 (c_{\sigma}^{\dagger} c_{\alpha\sigma} + h.c.) + U(n_{\uparrow} - \frac{1}{2})(n_{\downarrow} - \frac{1}{2}) \quad (19)$$

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.12 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) [288,289].

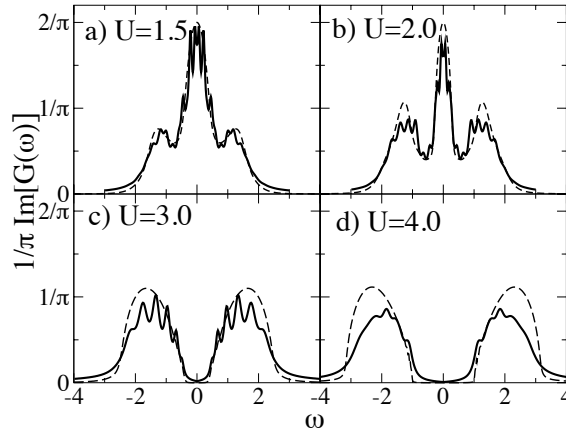


Fig. 12. Density of states ($\frac{1}{\pi} \text{Im}G(\omega)$) for the half-filled Hubbard Model. We also show the IPT results (dashed lines) (see text).

Results for the imaginary part of the Green’s functions 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.

As a conclusion, using DMRG as the impurity-solver of the DMFT, increases its performance. 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. [276] In addition, with this method, realistic band-structure calculations of systems with a larger number of degrees of freedom can be handled.

7. 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 a variety of fields such as Condensed Matter, Statistical Mechanics, High Energy Physics and Quantum Chemistry. It is still evolving and it presents very interesting potential new applications.

Among the fields where DMRG has still to be exploited are the time-dependent analysis of quantum and dissipative systems, the application in DMFT band-structure calculations and in quantum chemistry.

The connection of DMRG with quantum information theory paves the way to an important new field of application and, very possibly, to higher dimensions.

Acknowledgments

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References

1. S. White, Phys. Rev. Lett. **69**, 2863 (1992)
2. *Density Matrix Renormalization*, edited by I. Peschel, X. Wang, M. Kaulke and K. Hallberg (Series: Lecture Notes in Physics, Springer, Berlin, 1999)
3. U. Schollwöck, *The density matrix renormalization group*, to appear in Rev. Mod. Phys., Jan. 2005
4. S. White, Phys. Rev. B **48**, 10345 (1993)
5. J. Bray and S. Chui, Phys. Rev. B **19**, 4876 (1979)
6. C. Pan and X. Chen, Phys. Rev. B **36**, 8600 (1987); M. Kovarik, Phys. Rev. B **41**, 6889 (1990)
7. T. Xiang and G. Gehring, Phys. Rev. B **48**, 303 (1993)
8. K. Wilson, *Rev. Mod. Phys.* **47**, 773 (1975)
9. S. White and R. Noack, Phys. Rev. Lett. **68**, 3487, (1992); R. Noack and S. White, Phys. Rev. B **47**, 9243 (1993)
10. J. Gaite, Mod. Phys. Lett. A **16**, 1109 (2001)
11. R. Noack and S. White in Ref. [2], Chap. 2(I)
12. M. Martín-Delgado, G. Sierra and R. Noack, J. Phys. A: Math. Gen. **32**, 6079 (1999)
13. R. Feynman, *Statistical Mechanics: A Set of Lectures*, (Benjamin, Reading, MA, 1972)
14. S. R. White, I. Affleck and D. Scalapino, Phys. Rev. B **65**, 165122 (2002)
15. See E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994)
16. E. R. Davidson, J. Comput. Phys. **17**, 87 (1975); E.R. Davidson, *Computers in Physics* **7**, No. 5, 519 (1993).
17. T. Osborne and M. Nielsen, Quantum Information Processing, Volume 1, Issue 1-2, 45 (2002) (available on-line: <http://www.kluweronline.com/issn/1570-0755/>)
18. F. Verstraete and J. Cirac, preprint, cond-mat/0407066
19. F. Verstraete, D. Porras and C. Cirac, Phys. Rev. Lett. **93** 227205 (2004); J. Latorre, E. Rico and G. Vidal, Quant. Inf. Comp. **6**, 48 (2004); J. Gaite, Proceedings of the conference TH2002, quant-ph/0301120
20. S. White, Phys. Rev. Lett. **77**, 3633 (1996)
21. T. Nishino and K. Okunishi, Phys. Soc. Jpn. **64**, 4084 (1995); U. Schollwöck, Phys. Rev. B **58**, 8194 (1998) and Phys. Rev. B **59**, 3917 (1999) (Erratum).
22. Ö. Legeza and G. Fátth, Phys. Rev. B **53**, 14349 (1996); M-B Lepetit and G. Pastor, Phys. Rev. B **58**, 12691 (1998)

23. S. Östlund and S. Rommer, Phys. Rev. Lett. **75**, 3537 (1995); S. Rommer and S. Östlund, Phys. Rev. B **55**, 2164 (1997); M. Andersson, M. Boman and S. Östlund, Phys. Rev. B **59**, 10493 (1999); H. Takasaki, T. Hikihara and T. Nishino, J. Phys. Soc. Jpn. **68**, 1537 (1999); K. Okunishi, Y. Hieida and Y. Akutsu, Phys. Rev. E **59**, R6227 (1999)
24. M. A. Martín-Delgado and G. Sierra, Int. J. Mod. Phys. A, **11**, 3145 (1996)
25. G. Sierra and M. A. Martín-Delgado, in "The Exact Renormalization Group " by A. Krasnitz, R. Potting, Y. A. Kubyshin and P. S. de Sa (Eds.) World Scientific Pub Co; ISBN: 9810239394, (1999), (cond-mat/9811170)
26. I. Peschel, M. Kaulke and Ö. Legeza, Annalen der Physik **8**, 153 (1999), (cond-mat/9810174)
27. S. R. White and D. Huse, Phys. Rev. B **48**, 3844 (1993)
28. E. S. Sørensen and I. Affleck, Phys. Rev. B **49**, 13235 (1994)
29. E. S. Sørensen and I. Affleck, Phys. Rev. B **49**, 15771 (1994); E. Polizzi, F. Mila and E. Sørensen, Phys. Rev. B **58**, 2407 (1998)
30. C. Batista, K. Hallberg and A. Aligia, Phys. Rev. B **58**, 9248 (1998); Phys. Rev. B **60**, 12553 (1999); Physica B, **259**, 1017 (1999); E. Jannod, C. Payen, K. Schoumacker, C. Batista, K. Hallberg and A. Aligia, Phys. Rev. B, **62**, 2998 (2000)
31. M. Laukamp et al., Phys. Rev. B **5**, 10755 (1998)
32. T-K. Ng, J. Lou and Z. Su, Phys. Rev. B **61**, 11487 (2000)
33. J. Lou, S. Qin, T-K. Ng, Z. Su and I. Affleck, Phys. Rev. B **62**, 3786 (2000)
34. S-W Tsai and J. B. Marston, Ann. Phys. (Leipzig) **8**, Special Issue, 261 (1999)
35. M. Sieling, U. Löw, B. Wolf, S. Schmidt, S. Zvyagin and B. Lüthi, Phys. Rev. B **61**, 88 (2000)
36. Y. Nishiyama, K. Totsuka, N. Hatano and M. Suzuki, J. Phys. Soc. Jpn **64**, 414 (1995)
37. S. Qin, T. Ng and Z-B Su, Phys. Rev. B **52**, 12844 (1995)
38. U. Schollwöck and T. Jolicoeur, Europhys. Lett. **30**, 493 (1995)
39. X. Wang, S. Qin and Lu Yu, Phys. Rev. B. **60**, 14529 (1999)
40. W. Tatsuki, Phys. Rev. E **61**, 3199 (2000); T. Wada and T. Nishino, cond-mat/0103508 (Proceedings of the Conference on Computational Physics 2000 (CCP2000), Gold Coast, Queensland, Australia, 3-8 December 2000)
41. M. Capone and S. Caprara, Phys. Rev. B **64**, 184418 (2001)
42. J. Lou, X. Dai, S. Qin, Z. Su and L. Yu, Phys. Rev. B **60**, 52 (1999)
43. E. Ercolessi, G. Morandi, P. Pieri and M. Roncaglia, Europhys. Lett. **49**, 434 (2000)
44. S. Qin, X. Wang and Lu Yu, Phys. Rev. B **56**, R14251 (1997)
45. K. Hallberg, P. Horsch and G. Martínez, Phys. Rev. B, **52**, R719 (1995)
46. H. E. Boos, V. E. Korepin, Y. Nishiyama and M. Shiroishi, J. Phys. A **35**, 4443 (2002); V. E. Korepin, S. Lukyanov, Y. Nishiyama and M. Shiroishi, Phys. Lett. A **312**, 21 (2003)
47. M. Shiroishi, M. Takahashi and Y. Nishiyama, J. Phys. Soc. Jpn. **70**, 3535 (2001)
48. T. Hikihara and A. Furusaki, Phys. Rev. B **58**, R583 (1998)
49. G. Fath, Phys. Rev. B **68**, 134445 (2003)
50. J. Lou, S. Qin, C. Chen, Z. Su and L. Yu, Phys. Rev. B **65**, 064420 (2002)
51. J. Lou, S. Qin and C. Chen, Phys. Rev. Lett. **91**, 087204 (2003)
52. F. Capraro and C. Gros, Eur. Phys. J. B **29** 1, 35 (2002)
53. Y. Hieida, K. Okunishi and Y. Akutsu, Phys. Rev. B **64**, 224422 (2001)
54. T. Byrnes, R. Bursill, H-P. Eckle, C. Hamer and A. Sandvik, Phys. Rev. B **66**, 195313 (2002)
55. S-W. Tsai and J. B. Marston, Phys. Rev. B **62**, 5546 (2000)
56. K. Hallberg, X. Wang, P. Horsch and A. Moreo, Phys. Rev. Lett. **76**, 4955 (1996)
57. A. Moreo, Phys. Rev. B **35**, 8562 (1987); T. Ziman and H. Schulz, Phys. Rev. Lett **59**, 140 (1987)
58. Y. Yamashita, N. Shibata and K. Ueda, Phys. Rev. B **58**, 9114 (1998); Y. Yamashita, N. Shibata and K. Ueda, J. Phys. Soc. Jpn. **69**, 242 (2000); Y. Yamashita, N. Shibata and K. Ueda, Phys. Rev. B **61**, 4012 (2000)
59. A. Onufriev and B. Marston, Phys. Rev. B **59**, 12573 (1999)
60. C. Itoi, S. Qin and I. Affleck, Phys. Rev. B **61**, 6747 (2000)
61. W. Yu and S. Haas, Phys. Rev. B **63**, 024423 (2001)
62. R. J. Bursill, T. Xiang and G. A. Gehring, J. Phys. A **28** 2109 (1994)
63. R. J. Bursill, G. A. Gehring, D. J. J. Farnell, J. B. Parkinson, T. Xiang and C. Zeng, J. Phys. C **7** 8605 (1995)
64. U. Schollwöck, Th. Jolicoeur and T. Garel, Phys. Rev. B **53**, 3304 (1996)

65. R. Chitra, S. Pati, H. R. Krishnamurthy, D. Sen and S. Ramasesha, Phys. Rev. B **52**, 6581 (1995); S. Pati, R. Chitra, D. Sen, H. R. Krishnamurthy and S. Ramasesha, Europhys. Lett. **33**, 707 (1996); J. Malek, S. Drechsler, G. Paasch and K. Hallberg, Phys. Rev. B **56**, R8467 (1997); E. Sørensen et al in Ref. [2], Chap.1.2 (Part II) and references therein; D. Augier, E. Sørensen, J. Riera and D. Poilblanc, Phys. Rev. B **60**, 1075 (1999)
66. Y. Kato and A. Tanaka, J. Phys. Soc. Jpn. **63**, 1277 (1994)
67. S. R. White and I. Affleck, Phys. Rev. B **54**, 9862 (1996)
68. G. Bouzerar, A. Kampf and G. Japaridze, Phys. Rev. B **58**, 3117 (1998); G. Bouzerar, A. Kampf and F. Schönfeld, cond-mat/9701176, unpublished; M-B. Lepetit and G. Pastor, Phys. Rev. B **56**, 4447 (1997)
69. M. Kaburagi, H. Kawamura and T. Hikihara, J. Phys. Soc. Jpn. **68**, 3185 (1999)
70. T. Hikihara, J. Phys. Soc. Jpn. **71**, 319 (2002); T. Hikihara, M. Kaburagi, H. Kawamura and T. Tonegawa, Phys. Rev. B **63**, 174430 (2001)
71. S. Pati, S. Ramasesha and D. Sen, Phys. Rev. B **55**, 8894 (1996); J. Phys. Cond. Matt. **9**, 8707 (1997); T. Tonegawa, T. Hikihara, T. Nishino, M. Kaburagi, S. Miyashita, H.J. Mikeska, J. Mag. **177-181**, 647 (1998)
72. M. Azzouz, L. Chen and S. Moukouri, Phys. Rev. B **50** 6223 (1994); S. R. White, R. M. Noack and D. J. Scalapino, Phys. Rev. Lett. **73** 886 (1994); K. Hida, J. Phys. Soc. Jpn. **64** 4896 (1995); T. Narushima, T. Nakamura and S. Takada, J. Phys. Soc. Jpn. **64** 4322 (1995); U. Schollwöck and D. Ko, Phys. Rev. B **53** 240 (1996); G. Sierra, M. A. Martín-Delgado, S. White and J. Dukelsky, Phys. Rev. B **59**, 7973 (1999); S. White, Phys. Rev. B **53**, 52 (1996)
73. A. Kawaguchi, A. Koga, K. Okunishi and N. Kawakami, Phys. Rev. B **65**, 214405 (2002)
74. A. Trumper and C. Gazza, Phys. Rev. B **64**, 134408 (2001)
75. M. Roger, Phys. Rev. B **63**, 144433 (2001)
76. T. Hikihara and A. Furusaki, Phys. Rev. B **63**, 134438 (2001)
77. A. Laeuchli, G. Schmid and M. Troyer, Phys. Rev. B **67**, 100409 (2003)
78. T. Hikihara, T. Momoi and X. Hu, Phys. Rev. Lett. **90**, 087204 (2003)
79. T. Nunner, P. Brune, T. Kopp, M. Windt and M. Grüninger, Phys. Rev. B **66**, 180404 (2002)
80. Y. Honda and T. Horiguchi, preprint, cond-mat/0106426
81. S. K. Pati and R. R. P. Singh, Phys. Rev. B **60**, 7695 (1999); S. R. White and R. Singh, Phys. Rev. Lett. **85**, 3330 (2000)
82. N. Maeshima, M. Hagiwara, Y. Narumi, K. Kindo, T. C. Kobayashi and K. Okunishi, Journal of Physics: Cond. Matt. **15**, 3607 (2003); N. Maeshima and K. Okunishi, Phys. Rev. B **62**, 934-939 (2000)
83. C. Itoi and S. Qin, Phys. Rev. B **63**, 224423 (2001)
84. J. Lou, J. Dai, S. Qin, Z. Su and L. Yu, Phys. Rev. B **62**, 8600 (2000)
85. C. Raghui, I. Rudra, S. Ramasesha and D. Sen, Phys. Rev. B **62**, 9484 (2000)
86. A. Honecker, M. Kaulke and K.D. Schotte, Eur. Phys. J. B **15**, 423 (2000)
87. A. Gendiar and A. Surda, Phys. Rev. B **62**, 3960 (2000)
88. K. Tandon, S. Lal, Swapan K. Pati, S. Ramasesha and D. Sen, Phys. Rev. B **59**, 396 (1999); R. Citro, E. Orignac, N. Andrei, C. Itoi and S. Qin, J. Phys.: Cond. Mat. **12**, 3041 (2000)
89. J. Lou, C. Chen and S. Qin, Phys. Rev. B **64**, 144403 (2001)
90. X. Wang and L. Yu, Phys. Rev. Lett. **84**, 5399 (2000)
91. S. K. Pati, S. Ramasesha and D. Sen, in *Magnetism: Molecules to Materials IV*, eds. J.S. Miller and M. Drillon (Wiley-VCH Weinheim, 2002), Chapter 4, (cond-mat/0106621)
92. L. Chen and S. Moukouri, Phys. Rev. B **53** 1866 (1996); S. J. Qin, S. D. Liang, Z. B. Su and L. Yu, Phys. Rev. B **52** R5475 (1995); R. Noack in Ref. [2], Chap.1.3 (Part II); S. Daul and R. Noack, Phys. Rev. B **61**, 12361 (2000); M. Vojta, R. Hetzel and R. Noack, Phys. Rev. B **60**, R8417 (1999)
93. K. Penc, K. Hallberg, F. Mila and H. Shiba, Phys. Rev. Lett. **77**, 1390 (1996); Phys. Rev. B, **55**, 15475 (1997)
94. N. Bulut, Advances in Physics **51**, no. 6 (2002)
95. A. Malvezzi, T. Paiva and R. dos Santos, Phys. Rev. B **66**, 064430 (2002)
96. E. Jeckelmann, Phys. Rev. Lett. **89**, 236401 (2002)
97. Y. Zhang, C. Wu and H. Q. Lin, Phys. Rev. B **65**, 115101 (2002)
98. C. Aebischer, D. Baeriswyl and R. M. Noack, Phys. Rev. Lett. **86**, 468 (2001)
99. R. Arita and H. Aoki, Phys. Rev. B **61**, 12261 (2000); R. Arita, Y. Shimoi, K. Kuroki and H. Aoki, Phys. Rev. B **57**, 10609 (1998)
100. S. Daul, Eur. J. Phys. B **14**, 649 (2000)

101. S. Qin, J. Lou, T. Xiang, G-S. Tian and Z. Su, Phys. Rev. B **68**, 045110 (2003)
102. A. Aligia, K. Hallberg, C. Batista and G. Ortiz, Phys. Rev. B **61**, 7883 (2000)
103. V. Meden, W. Metzner, U. Schollwoeck, O. Schneider, T. Stauber and K. Schoenhammer, Europhys. J B **16**, 631 (2000)
104. P. Farkasovsky, Phys. Rev. B **65**, 081102 (2002)
105. C. Schuster, R. Roemer and M. Schreiber, Phys. Rev. B **65**, 115114 (2002)
106. K. Hida, Phys. Rev. Lett. **86**, 1331 (2001)
107. W. Lay and J. Rudnick, Phys. Rev. Lett. **88**, 057203 (2002); Y. Nishiyama, J. Phys. A **34**, 11215 (2001); S. G. Chung, Phys. Rev. E **62**, 3262 (2000)
108. B. Srinivasan and M. B. Lepetit, Phys. Rev. B **66**, 024421 (2002); H. Sakamoto, T. Momoi and K. Kubo, Phys. Rev. B **65**, 224403 (2002)
109. K. Hamacher, C. Gros and W. Wenzel, Phys. Rev. Lett. **88**, 217203 (2002)
110. M. Vojta, A. Huebsch and R. M. Noack, Phys. Rev. B **63**, 045105 (2001); Z. Weihong, J. Oitmaa, C.J. Hamer and R.J. Bursill, J. Phys. C **13**, 433 (2001)
111. Youngho Park, S. Liang and T. K. Lee, Phys. Rev. B **59**, 2587 (1999)
112. S. Rommer, S. R. White and D. J. Scalapino, Phys. Rev. B **61**, 13424 (2000)
113. R. M. Noack, S. R. White and D. J. Scalapino, Phys. Rev. Lett. **73**, 882 (1994); S. R. White, R. M. Noack and D. J. Scalapino, J. Low Temp. Phys. **99**, 593 (1995); R. M. Noack, S. R. White and D. J. Scalapino, Europhys. Lett. **30**, 163 (1995); C. A. Hayward, D. Poilblanc, R. M. Noack, D. J. Scalapino and W. Hanke, Phys. Rev. Lett. **75**, 926 (1995); S. White and D. Scalapino, Phys. Rev. Lett. **81**, 3227 (1998); E. Jeckelmann, D. Scalapino and S. White, Phys. Rev. B **58**, 9492 (1998)
114. S. Nishimoto, E. Jeckelmann and D. Scalapino, Phys. Rev. B **66**, 245109 (2002)
115. J. B. Marston, J. O. Fjærestad and A. Sudbo, Phys. Rev. Lett. **89**, 056404 (2002)
116. U. Schollwoeck, S. Chakravarty, J. O. Fjærestad, J. B. Marston and M. Troyer, Phys. Rev. Lett. **90**, 186401 (2003)
117. L. G. Caron and C. Bourbonnais, Phys. Rev. B **66**, 045101 (2002)
118. G. Fano, F. Ortolani, A. Parola and L. Ziosi, Phys. Rev. B **60**, 15654 (1999)
119. N. Shibata and D. Yoshioka, Phys. Rev. Lett. **86**, 5755 (2001); Physica E **12**, 43 (2002) D. Yoshioka and N. Shibata, J. Phys. Soc. Jpn. **70**, 3690 (2001)
120. V. Meden and U. Schollwoeck, Phys. Rev. B **67**, 035106 (2003)
121. S. Liang and H. Pang, Europhys. Lett. **32**, 173 (1995)
122. S. White and D. Scalapino, Phys. Rev. B **55**, 14701 (1997)
123. S. White and D. Scalapino, Phys. Rev. B **55**, 6504 (1997)
124. S. White and D. Scalapino, Phys. Rev. B **57**, 3031 (1998)
125. E. Arrigoni, A. P. Harju, W. Hanke, B. Brendel and S.A. Kivelson, Phys. Rev. B **65**, 134503 (2002); J. Bonca, J. E. Gubernatis, M. Guerrero, E. Jeckelmann and S. R. White, Phys. Rev. B **61**, 3251 (2000); A. L. Chernyshev, S. White and A. H. Castro Neto, Phys. Rev. B, **65**, 214527 (2002); S. White and D. Scalapino, Phys. Rev. B **61**, 6320 (2000)
126. S. White and D. Scalapino, Phys. Rev. Lett. **80**, 1272 (1998); *ibid.* Phys. Rev. B **61**, 6320 (2000)
127. I. P. McCulloch, A. R. Bishop and M. Gulacsi, Phil. Mag. B **81**, 1603 (2001)
128. S. R. White and I. Affleck, Phys. Rev. B **64**, 024411 (2001)
129. T. Xiang, J. Lou and Z. Su, Phys. Rev. B **64**, 104414 (2001); P. Henelius, Phys. Rev. B **60**, 9561 (1999)
130. S. Nishimoto, E. Jeckelmann, F. Gebhard and R. Noack, Phys. Rev. B **65**, 165114 (2002)
131. N. Maeshima, Y. Hieida, Y. Akutsu, T. Nishino and K. Okunishi, Phys. Rev. E **64** (2001) 016705
132. M.A. Martin-Delgado, J. Rodriguez-Laguna and G. Sierra, Nucl. Phys. B **601**, 569 (2001)
133. P. Henelius, Phys. Rev. B **60**, 9561 (1999)
134. S. Moukouri and L. G. Caron, Phys. Rev. B **67**, 092405 (2003)
135. T. A. Costi, P. Schmitteckert, J. Kroha and P. Wölfle, Phys. Rev. Lett. **73**, 1275 (1994); S. Eggert and I. Affleck, Phys. Rev. Lett. **75**, 934 (1995); E. S. Sørensen and I. Affleck, Phys. Rev. B **51**, 16115 (1995); X. Q. Wang and S. Mallwitz, Phys. Rev. B **53**, R492 (1996); W. Wang, S. J. Qin, Z. Y. Lu, L. Yu and Z. B. Su, Phys. Rev. B **53**, 40 (1996); C. C. Yu and M. Guerrero, Phys. Rev. B **54**, 15917 (1996); A. Furusaki and T. Hikihara, Phys. Rev. B **58**, 5529 (1998)
136. K. Hallberg and R. Egger, Phys. Rev. B **55**, 8646 (1997)
137. C. Schuster and U. Eckern, Ann. Phys. (Leipzig) **11**, 901-915 (2002); W. Zhang, J. Igarashi and P. Fulde, Phys. Rev. B **56**, 654 (1997)

138. V. Meden, W. Metzner, U. Schollwoeck and K. Schoenhammer, Phys. Rev. B **65**, 045318 (2002)
139. C. C. Yu and S. R. White, Phys. Rev. Lett. **71**, 3866 (1993); C. C. Yu and S. R. White, Physica B **199**, 454 (1994)
140. S. Moukouri and L. G. Caron, Phys. Rev. B **52**, 15723 (1995); N. Shibata, T. Nishino, K. Ueda and C. Ishii, Phys. Rev. B **53**, R8828 (1996); M. Guerrero and R. M. Noack, Phys. Rev. B **53**, 3707 (1996)
141. H. Otsuka and T. Nishino, Phys. Rev. B **52**, 15066 (1995); S. Moukouri, L. G. Caron, C. Bourbonnais and L. Hubert, Phys. Rev. B **51**, 15920 (1995)
142. J. C. Xavier, E. Novais and E. Miranda, Phys. Rev. B **65**, 214406 (2002)
143. T. Yamamoto, R. Manago and Y. Mori, J. Phys. Soc. Jpn. **72**, 3204 (2003)
144. I. P. McCulloch, A. Juezapavicius, A. Rosengren and M. Gulacsi, Phys. Rev. B **65**, 052410 (2002)
145. M. Guerrero and R.M. Noack, Phys. Rev. B **63**, 144423 (2001)
146. S. Watanabe, J. Phys. Soc. Jpn. **69**, 2947 (2000)
147. I. P. McCulloch, M. Gulacsi, S. Caprara and A. Juezapavicius, J. Low Temp. Phys. **117**, 323 (1999)
148. J. Xavier, R. Pereira, E. Miranda and I. Affleck, Phys. Rev. Lett. **90**, 247204 (2003)
149. S. Watanabe, Y. Kuramoto, T. Nishino and N. Shibata, J. Phys. Soc. Jpn **68**, 159 (1999)
150. J. Moreno, S. Qin, P. Coleman and L. Yu, Phys. Rev. B **64**, 085116 (2001)
151. S. Moukouri, L. Chen and L. G. Caron, Phys. Rev. B **53**, R488 (1996)
152. J. Riera, K. Hallberg and E. Dagotto, Phys. Rev. Lett. **79**, 713 (1997); E. Dagotto et al., Phys. Rev. B **58**, 6414 (1998)
153. D. García, K. Hallberg, C. Batista, M. Avignon and B. Alascio, Phys. Rev Lett., **85**, 3720 (2000); D. J. García, K. Hallberg, C. D. Batista, S. Capponi, D. Poilblanc, M. Avignon and B. Alascio, Phys. Rev. B. **65**, 134444 (2002)
154. B. Ammon and M. Imada, J. Phys. Soc. Jpn. **70**, 547 (2001)
155. D. García, K. Hallberg, C. Batista, M. Avignon and B. Alascio, Phys. Rev Lett., **85**, 3720 (2000); D. García, K. Hallberg, B. Alascio and M. Avignon, Physical Rev. Lett., **93**, 17, 177204 (2004)
156. I.P. McCulloch, A. Juezapavicius, A. Rosengren and M. Gulacsi, Phys. Rev. B, **65**, 52410 (2002)
157. S. Ramasesha, S. Pati, H. R. Krishnamurthy, Z. Shuai and J. L. Brédas, Phys. Rev. B **54**, 7598 (1996); S. Ramasesha, S. Pati, H. R. Krishnamurthy, Z. Shuai and J. L. Brédas, Synth. Metals **85**, 1019 (1997)
158. E. S. Sørensen and I. Affleck, Phys. Rev. B **51**, 16115 (1995)
159. I. McCulloch and M. Gulacsi, Europhys. Lett. **57**, 852 (2002)
160. G. Sierra and T. Nishino, Nucl. Phys. B **495**, 505 (1997) (cond-mat/9610221)
161. T. Xiang, Phys. Rev. B **53**, R10445 (1996)
162. M.S.L. du Croo de Jongh and J.M.J. van Leeuwen, Phys. Rev. B **57**, 8494 (1998)
163. M-B. Lepetit, M. Cousy and G. Pastor, Eur. Phys. J. B **13**, 421 (2000); H. Otsuka, Phys. Rev. B **53**, 14004 (1996)
164. J. Dukelsky and G. Dussel, Phys. Rev. B **59**, R3005 (1999) and references therein.
165. J. Dukelsky and G. Sierra, Phys. Rev. Lett. **83**, 172 (1999)
166. J. Dukelsky and S. Pittel, Rep. Prog. Phys. **67**, 513 (2004)
167. M. A. Martín-Delgado and G. Sierra, Phys. Rev. Lett. **83**, 1514 (1999)
168. S. Glazek and K. Wilson, Phys. Rev. D **48**, 5863 (1993); **49**, 4214 (1994)
169. T. Eller, H.-C. Pauli and S. Brodsky, Phys. Rev. D **35**, 1493 (1987)
170. T. Nishino, J. Phys. Soc. Jpn. **64**, 3598 (1995); see also T. Nishino in Ref. [2], Chap. 5(I); T. Nishino and K. Okunishi in *Strongly Correlated Magnetic and Superconducting Systems*, Ed. G. Sierra and M. A. Martín-Delgado (Springer, Berlin, 1997)
171. H. Trotter, Proc. Am. Math. Soc. **10**, 545 (1959); M. Suzuki, Prog. Theor. Phys. **56**, 1454 (1976); R. Feynman and A. Hibbs *Quantum Mechanics and Path Integrals* (McGraw-Hill, 1965)
172. R. Bursill, T. Xiang and G. Gehring, J. Phys. Cond. Mat. **8**, L583 (1996); X. Q. Wang and T. Xiang, Phys. Rev. B **56**, 5061 (1997); N. Shibata, J. Phys. Soc. Jpn **66** 2221 (1997)
173. A. Gendiar and A. Surda, Phys. Rev. B **63**, 014401 (2001)
174. T. Nishino and N. Shibata, J. Phys. Soc. Jpn. **68**, 3501 (1999); T. Enss and U. Schollwoeck, J. Phys. A **34**, 7769 (2001)
175. A. Kemper, A. Schadschneider and J. Zittartz, J. Phys. A: Math. Gen. **34**, L279 (2001); T. Enss and U. Schollwöck, J Phys A: Math. Gen. **34**, 7769 (2001)
176. R. Baxter, J. Math. Phys. **9**, 650 (1968); J. Stat Phys. **19**, 461 (1978)
177. T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. **65**, 891 (1996); T. Nishino and K. Okunishi, J. Phys. Soc.

- Jpn. **66**, 3040 (1997); T. Nishino, K. Okunishi and M. Kikuchi, Phys. Lett. A **213**, 69 (1996)
178. H. Takasaki, T. Nishino and Y. Hieida, J. Phys. Soc. Jpn. **70**, 1429 (2001)
 179. T. Nishino, Y. Hieida, K. Okunishi, N. Maeshima, Y. Akutsu and A. Gendiar, Prog. Theor. Phys. **105**, 409 (2001)
 180. C. Ritter and G. von Gehlen, in "Quantization, Gauge Theory and Strings", ed. A. Semikhatov et al., Vol. I, p.563-578, Scientific World Pub. Co. (2001) (cond-mat/0009255)
 181. T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. **67**, 3066 (1998); T. Nishino, K. Okunishi, Y. Hieida, N. Maeshima and Y. Akutsu, Nucl. Phys. B **575**, 504 (2000)
 182. E. Carlon and A. Drzewiński, Phys. Rev. Lett. **79**, 1591 (1997); E. Carlon and A. Drzewiński, Phys. Rev. E **57**, 2626 (1998); E. Carlon, A. Drzewiński and J. Rogiers, Phys. Rev. B **58**, 5070 (1998); A. Drzewiński, A. Ciach and A. Maciolek, Eur. Phys. J. B **5**, 825 (1998); A. Maciolek, A. Ciach and A. Drzewiński, Phys. Rev. E **60**, 2887 (1999)
 183. A. Drzewinski, A. Maciolek and R. Evans, Phys. Rev. Lett. **85**, 3079 (2000); A. Drzewinski, Phys. Rev. E **62**, 4378 (2000)
 184. M.-C. Chung, M. Kaulke, I. Peschel, M. Pleimling and W. Selke, Eur. Phys. J. B **18**, 655 (2000)
 185. E. Carlon and F. Iglói, Phys. Rev. B **57**, 7877 (1998); F. Iglói and E. Carlon, Phys. Rev. B **59**, 3783 (1999); E. Carlon, C. Chatelain and B. Berche, Phys. Rev. B **60**, 12974 (1999)
 186. J. Kondev and J. Marston, Nucl. Phys. B **497**, 639 (1997); T. Senthil, B. Marston and M. Fisher, Phys. Rev. B **60**, 4245 (1999); J. Marston and S. Tsai, Phys. Rev. Lett. **82**, 4906 (1999); S. Tsai and J. Marston, Ann. Phys. (Leipzig) **8**, Special Issue, 261(1999)
 187. M. Kaulke and I. Peschel, Eur. Phys. J. B **5**, 727 (1998)
 188. Y. Hieida, J. Phys. Soc. Jpn. **67**, 369 (1998)
 189. I. Peschel and M. Kaulke, in Ref. [2], Chap. 3.1(II)
 190. E. Carlon, M. Henkel and U. Schollwöck, Eur. Phys. J. B **12**, 99(1999); E. Carlon, M. Henkel and U. Schollwoeck, Phys. Rev. E **63**, 036101 (2001)
 191. J. Hooyberghs, E. Carlon and C. Vanderzande, Phys. Rev. E **62**, 036124 (2001)
 192. S.G. Chung, Phys. Rev. B **60**, 11761(1999)
 193. R. Bursill, T. Xiang and G. Gehring, J. Phys. C **8**, L583 (1996)
 194. H. Trotter, Proc. Am. Math. Soc. **10**, 545 (1959); M. Suzuki, Prog. Theor. Phys. **56**, 1454 (1976)
 195. X. Wang and T. Xiang, Phys. Rev. B **56**, 5061 (1997)
 196. N. Shibata and K. Ueda, J. Phys. Soc. Jpn. Vol.70, 3690 (2001)
 197. N. Shibata, J. Phys. Soc. Jpn. **66**, 2221 (1997)
 198. N. Shibata, J. Phys. A, **36** 381 (2003)
 199. T. Xiang, Phys. Rev. B **58**, 9142 (1998)
 200. N. Shibata, B. Ammon, T. Troyer, M. Sigrist and K. Ueda, J. Phys. Soc. Jpn. **67**, 1086 (1998)
 201. K. Maisinger, U. Schollwöck, S. Brehmer, H-J. Mikeska and S. Yamamoto, Phys. Rev. B **58**, R5908 (1998)
 202. S. Rommer and S. Eggert, Phys. Rev. B **59**, 6301 (1999)
 203. I. Maruyama, N. Shibata and K. Ueda, Phys. Rev. B **65**, 174421 (2002)
 204. K. Maisinger and U. Schollwöck, Phys. Rev. Lett. **81**, 445 (1999)
 205. B. Ammon, M. Troyer, T. Rice and N. Shibata, Phys. Rev. Lett. **82**, 3855 (1999); N. Shibata and H. Tsunetsugu, J. Phys. Soc. Jpn. **68**, 3138 (1999)
 206. F. Naef and X. Wang, Phys. Rev. Lett. **84**, 1320 (2000)
 207. A. Klümper, R. Raupach and F. Schönhofeld, Phys. Rev. B **59**, 3612 (1999)
 208. S. Moukouri and L. Caron, Phys. Rev. Lett. **77**, 4640 (1996).
 209. S. Moukouri and L. Caron, see Ref. [2], Chap. 4.5(II)
 210. S. Moukouri, preprint, cond-mat/0011169
 211. W. Zhang, J. Igarashi and P. Fulde, J. Phys. Soc. Jpn. **66**, 1912 (1997)
 212. L. Caron and S. Moukouri, Phys. Rev. Lett. **76**, 4050 (1996); L. Caron and S. Moukouri, Phys. Rev. B **56**, R8471 (1997)
 213. E. Jeckelmann and S. White, Phys. Rev. B **57**, 6376 (1998)
 214. R. Noack, S. White and D. Scalapino in *Computer Simulations in Condensed Matter Physics VII*, edited by D. Landau, K.-K. Mon and H.-B. Schüttler (Springer Verlag, Heidelberg and Berlin, 1994)
 215. E. Jeckelmann, C. Zhang and S. White in Ref. [2], Chap. 5.1 (II)
 216. C. Zhang, E. Jeckelmann and S. White, Phys. Rev. Lett. **80**, 2661 (1998); E. Jeckelmann, C. Zhang and S. R. White, Physical Review B **60**, 7950 (1999)

217. Y. Nishiyama, Phys. Rev. B **64**, 064510 (2001)
218. Y. Nishiyama, Eur. Phys. J. B **12**, 547 (1999)
219. R. Bursill, Y. McKenzie and C. Hammer, Phys. Rev. Lett. **80**, 5607 (1998); R. Bursill, Y. McKenzie and C. Hammer, Phys. Rev. Lett. **83**, 408 (1999); R. Bursill, Phys. Rev. B **60**, 1643 (1999)
220. R. Pai, R. Pandit, H. Krishnamurthy and S. Ramasesha, Phys. Rev. Lett. **76**, 2937 (1996) (see also the comment by N. V. Prokof'ev and B. V. Svistunov, Phys. Rev. Lett. **80**, 4355 (1998)); S. Rapsch, U. Schollwöck and W. Zwerger, Europhys. Lett. **46**, 559 (1999)
221. T. Kühner and H. Monien, Phys. Rev. B **58**, R14741 (1998)
222. I. Peschel and M-C. Chung, J. Phys. A: Math. Gen. **32**, 8419 (1999)
223. P. Maurel and M-B. Lepetit, Phys. Rev. B **62**, 10744 (2000); P. Maurel, M-B. Lepetit and D. Poilblanc, Eur. Phys. J. B **21**, 481 (2001)
224. K. Hida, J. Phys. Soc. Jpn. **65**, 895 (1996) and 3412 (1996) (erratum); J. Phys. Soc. Jpn. **66**, 330 (1997); J. Phys. Soc. Jpn. **66**, 3237 (1997); Prog. Theor. Phys. Suppl. **145**, 320 (2002)
225. K. Hida, J. Phys. Soc. Jpn. **68**, 3177 (1999)
226. K. Hida, Phys. Rev. Lett. **83**, 3297 (1999)
227. F. Igloi, R. Juhasz and P. Lajko, Phys. Rev. Lett. **86**, 1343 (2001)
228. R. Mélin, Y-C. Lin, P. Lajkó, H. Rieger and F. Igloi, Phys. Rev. B **65**, 104415 (2002)
229. P. Schmitteckert, T. Schulze, C. Schuster, P. Schwab and U. Eckern, Phys. Rev. Lett. **80**, 560 (1998); P. Schmitteckert and U. Eckern, Phys. Rev. B **53**, 15397 (1996)
230. D. Weinmann, P. Schmitteckert, R. Jalabert and J. Pichard, Eur. Phys. J. B **19**, 139-156 (2001)
231. P. Schmitteckert, R. Jalabert, D. Weinmann and J. L. Pichard, Phys. Rev. Lett. **81**, 2308 (1998)
232. E. Carlon, P. Lajko and F. Igloi, Phys. Rev. Lett. **87**, 277201 (2001)
233. G. Fano, F. Ortolani and L. Ziosi, J. Chem. Phys. **108**, 9246 (1998), (cond-mat/9803071); R. Bursill and W. Barford, Phys. Rev. Lett. **82**, 1514 (1999)
234. M. Exler and J. Schnack, Phys. Rev. B **67**, 094440 (2003)
235. B. Normand, X. Wang, X. Zotos and Daniel Loss, Phys. Rev. B **63**, 184409 (2001)
236. C. Raghu, Y. Anusooya Pati and S. Ramasesha, Journal-ref: J. Phys. A **34**, 11215 (2001)
237. W. Barford and R. Bursill, Chem. Phys. Lett. **268**, 535 (1997); W. Barford, R. Bursill and M. Lavrentiev, J. Phys: Cond. Matt, **10**, 6429 (1998); W. Barford in Ref. [2], Chap.2.3 (Part II) and references therein; M. Lavrentiev, W. Barford, S. Martin, H. Daly, R. Bursill, Physical Review B **59**, 9987 (1999)
238. E. Carlon, A. Drzewinski and J. van Leeuwen, J. Chem. Phys. **117**, 2425 (2002); Phys. Rev. E **64**, 010801(R) (2001); M. Paessens and G. Schütz, Phys. Rev. E **66**, 021806 (2002);
239. M. A. Martín-Delgado, J. Rodriguez-Laguna and G. Sierra, Phys. Rev. B **65**, 155116 (2002)
240. S. White and R. Martin, J. Chem. Phys. **110**, 4127 (1999); see also S. White in [2], Chap. 2.1.
241. S. White in Ref. [2], Chap. 2.1.
242. Ö. Legeza, J. Röder and B.A. Hess, Phys. Rev. B **67**, 125114 (2003)
243. S. Daul, I. Ciofini, C. Daul and S. R. White, In. J. Quantum Chem. **79**, 331 (2000)
244. C. Bauschlicher and P. Taylor, J. Chem. Phys. **85**, 2779 (1986)
245. Ö. Legeza, J. Roder and B. A. Hess, Phys. Rev. B **67**, 125114 (2003)
246. M. A. Cazalilla and J. B. Marston, Phys. Rev. Lett. **88**, 256403 (2002)
247. P. Schmitteckert, Phys. Rev. B **70**, 121302 (2004)
248. H. G. Luo, T. Xiang and X. Q. Wang, Phys. Rev. Lett. **91**, 049701 (2003) (comment to [246]); M. A. Cazalilla and J. B. Marston, Phys. Rev. Lett. **91**, 049702 (2003) (response to previous comment)
249. S. White and A. Feiguin, Phys. Rev. Lett. **93**, 076401 (2004)
250. A. Daley et al., J. Stat. Mech.: Theor. Exp. P04005 (2004)
251. G. Vidal, Phys. Rev. Lett. **91**, 147902 (2003); G. Vidal, Phys. Rev. Lett. **93**, 040502 (2004)
252. K. Hallberg, Phys. Rev. B **52**, 9827 (1995).
253. T. Kühner and S. White, Phys. Rev. B **60**, 335 (1999)
254. Y. Anusooya, S. Pati and S. Ramasesha, J. Chem. Phys. **106**, 1 (1997); S. Ramasesha, K. Tandon, Y. Anusooya and S. Pati, Proc. of SPIE, **3145**, 282 (1997); S. Ramasesha, Z. Shuai and J. Brédas, Chem. Phys. Lett. **245**, 224 (1995)
255. E. Jeckelmann, Phys. Rev. B **66**, 045114 (2002)
256. W. Hofstetter, Phys. Rev. Lett. **85**, 1508 (2000)
257. E. R. Gagliano and C. A. Balseiro, Phys. Rev. Lett. **59**, 2999 (1987).
258. G. Grosso and G. Partori Parravicini, in *Memory Function Approaches to Stochastic Problems in Condensed*

- Matter*, Adv. in Chemical Physics, **62**, 133 (Wiley, N. Y., 1985)
259. P. Horsch and W. von der Linden, *Z. Phys. B* **72** 181 (1981)
260. Y. Nishiyama, *Eur. J. Phys. B* **12**, 547 (1999)
261. C. L. Zhang, E. Jeckelmann and S. White, *Phys. Rev. B* **60**, 14092 (1999)
262. W. Q. Yu and S. Haas, *Phys. Rev. B*, **63**, 024423 (2000)
263. K. Okunishi, Y. Akutsu, N. Akutsu and T. Yamamoto, *Phys. Rev. B* **64**, 104432 (2001)
264. T. Nunner, P. Brune, T. Kopp, M. Windt and M. Grüninger, *Phys. rev. B* **66**, 180404
265. K. Penc, K. Hallberg, F. Mila and H. Shiba, *Phys. Rev. Lett.* **77**, 1390 (1996); K. Penc, K. Hallberg, F. Mila and H. Shiba, *Phys. Rev. B*, **55**, 15475 (1997)
266. S. S. Kancharla and C. J. Bolech, *Phys. Rev. B* **64**, 085119 (2001)
267. F. Essler, F. Gebhard and E. Jeckelmann, *Phys. Rev. B* **64**, 125119 (2001); E. Jeckelmann, F. Gebhard and F. Essler, *Phys. Rev. Lett.* **85**, 3910 (2000)
268. E. Jeckelmann, *Phys. Rev. B* **67**, 075106 (2003)
269. Y.-J Kim, J. P. Hill, H. Benthien, F. H. L. Essler, E. Jeckelmann, H. S. Choi, T. W. Noh, N. Motoyama, K. M. Kojima, S. Uchida, D. Casa, and T. Gog *Phys. Rev. Lett.* **92**, 137402 (2004)
270. S. K. Pati and R. Singh, *Phys. Rev. B* **60**, 7695 (1999)
271. T. D. Kühner, S. White and H. Monien, *Phys. Rev. B* **61**, 12474 (2000)
272. C. Raas, G. Uhrig and F. B. Anders, *Phys. Rev. B* **69**, 041102(R) (2004)
273. X. Wang, K. Hallberg and F. Naef in Ref. [2], Chap.7(I)
274. T. Mutou, N. Shibata and K. Ueda, *Phys. Rev. Lett* **81**, 4939 (1998) (erratum: *Phys. Rev. Lett.* **82**, 3727 (1999))
275. F. Naef, X. Wang, X. Zotos and W. von der Linden, *Phys. Rev. B* **60**, 359 (1999)
276. G. Kotliar and D. Vollhardt, *Physics Today* **57**, 53 (2004)
277. J.E. Hirsch and R.M. Fye, *Phys. Rev. Lett.* **56**, 2521 (1986)
278. M.J. Rozenberg, *Phys. Rev. B* **55**, R4855 (1997)
279. K. G. Wilson, *Rev. Mod. Phys.* **47**, 773 (1975)
280. R. Bulla, *Phys. Rev. Lett.* **83**, 136 (1999)
281. R. Bulla, T. Costi and D. Vollhardt, *Phys. Rev. B* **64**, 045103 (2001)
282. D. García, K. Hallberg and M. Rozenberg, *Phys. Rev. Lett.* **93**, 246403 (2004)
283. A. Georges, G. Kotliar, Werner Krauth and Marcelo J. Rozenberg *Rev. Mod. Phys.* **68**, 13 (1996)
284. Q. Si, M. J. Rozenberg, G. Kotliar, and A. E. Ruckenstein *Phys. Rev. Lett.* **72**, 2761 (1994)
285. M. J. Rozenberg, G. Moeller and G. Kotliar, *Mod. Phys. Lett. B* **8**, 535 (1994)
286. See F. Gebhard, E. Jeckelmann, S. Mahler, S. Nishimoto and R. Noack, *Eur. Phys. J B* **36**, 491 (2003), for a previous attempt using a particular algorithm of the DMRG restricted to the small U metallic regime.
287. S. Nishimoto, F. Gebhard and E. Jeckelmann, *J. Phys.: Cond. Matt.* **16**, 7063, (2004)
288. A. Georges and G. Kotliar, *Phys. Rev. B* **45**, 6479 (1992)
289. X. Y. Zhang, M. J. Rozenberg and G. Kotliar, *Phys. Rev. Lett.* **70**, 1666 (1993), A. Georges and W. Krauth *Phys. Rev. B* **48**, 7167-7182 (1993).