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Application of density matrix renormalization group to one-dimensional Hubbard model to study strongly correlated electrons system

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In this work, we applied density matrix renormalization group to one-dimensional Hubbard model at five numbers of sweep to solve strongly correlated interacting electrons system, starting from two electrons on two sites up to ten electrons on ten sites at half filling. The results that emerged from the present study is in agreement with that of exact diagonalization, variational and Lanczos solution at the varying values of the Coulomb interaction strength (*U/t*) at *t*=1. The total energy, E_g/t, of the ground state increases with the increase in interaction strength for all the numbers of site, *N*. The spectra intensity increases with increase in the interaction strength but decreases to zero when the interaction strength is made negatively large. This study is extended to more than two electrons on two sites. We equally show effect of interaction strength, *U/t*, at *t* = 1 on the energy-dependent entropy, *S*.

Key words: Density matrix renormalization group, Hubbard model, sweep, exact diagonalization, variational, Lanczos, entropy.

INTRODUCTION

The Hubbard model (Hubbard, 1963) has been greatly considered to be the basic formalism for tackling electron-electron correlations in interacting many-body systems ever since the advent of high-T_c super-conductors. This model captures the dominant competition between the delocalizing effects of the kinetic energy and the localizing effects of the electron-electron repulsion. In spite of the simple form of this model, it has provided meaningful insights into the many-body properties, like high-T_c superconductivity, metal-insulator transitions and magnetic states of solids.

Strong interactions between the electrons in many materials of technological interest, lead to collective behavior. The study of these strongly correlated electrons systems has turned out to be the core area of research especially in condensed matter physics and display a broad range of vital phenomena (Alvarez et al., 2007). In this context, Hamiltonian models are used to simulate the relevant interactions of a given compound, and the relevant degrees of freedom. The dependence of these studies is on the use of tight-binding lattice models that consider electron localization, where states on one site

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can be labeled by spin and orbital degrees of freedom.

Examples of these models include the Hubbard model (Hubbard, 1963, 1964), the *t-J* model (Spalek, 1977, 2007) and the spin 1/2 Heisenberg model, which can be considered the undoped limit of the *t-J* model.

There are many different ways to simplify the calculations for strongly correlated systems and one such method is the DMRG, invented by White in 1992. The DMRG is a numerical variational technique to study quantum many-body Hamiltonians that could be classified as a diagonalization method. In the past decade, the DMRG algorithm invented by White (1992) has been proven strongly to be successful for calculating the ground state properties of model Hamiltonians for very large systems in one dimension. In recent years, it has been adopted to study coupled fermionic and spin chain. It was even introduced to organic ferromagnets (Liu et al., 2004) when it was reformulated to models defined in momentum space (Xiang, 1996).

For one dimensional system, this method can truncate, with bounded errors and in a general and efficient way, the underlying Hilbert space to a constant size. The detailed explanation of this technique (DMRG) cannot be captured in this present research paper, and we will only provide a brief procedural description of the method. The original paper (White, 1992) along with many published reviews (Hallberg, 2006; Rodriguez-Laguna, 2002; Schollwöck, 2005) are highly recommended for physicists who are not familiar with the technique.

The present paper and accompanying code can be used in different ways. Physicists will be able to immediately use the flexible input file to run the code for the Hubbard model with inhomogeneous couplings, Hubbard *U* values, and on-site potentials, as well as different symmetries, either on one-dimensional chains or on *n*-leg ladders. Readers with knowledge of DMRG and C++ will be able to understand the implementation of the algorithm.

Other software projects, such as the ALPS project also implement the DMRG algorithm within their own frameworks. However, this paper emphasizes on the computational approach to study strongly correlated electron systems.

In this paper, we studied the one-dimensional (1-D) Hubbard model starting with two electrons on two sites up to ten electrons on ten sites. We employed the DMRG method (White, 1992) with the implementation of ITensor code (written in C++ programming language) (ITENSOR library, http://itensor.org) in order to solve the ground state in such complicated systems as precisely as possible. Especially, we concentrate on half-filling cases, in which many theoretical treatments failed to predict.

By applying DMRG to 1-D Hubbard model, using some intrinsic routines in ITENSOR DMRG, we present the ground state energy for *N* electrons on *N* sites with $2 \leq N \leq 10$. The maximum entropy with respect to interaction strength is also presented.

METHODOLOGY

Model and parameters

The single band Hubbard Hamiltonian is written as

$$H = -t \sum_{<i,j>\sigma} \left(c_{i\sigma}^{+} c_{j\sigma} + h.c\right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \quad (1)$$

where $\langle i,j \rangle$ denotes nearest-neighbour (*NN*) sites, $c_{i\sigma}^{+}$ ($c_{j\sigma}$) is the creation (annihilation) operator with spin $\sigma = \uparrow$ or $\downarrow$ at site *i,* and $n_{i\sigma} = c_{i\sigma}^{+} c_{j\sigma}$ is the occupation number operator, and of course *h.c* is the Hermitian conjugate. The transfer integral t_{ij} is written as $t_{ij} = t$, meaning that all hopping processes have the same probability. The parameter, *U* is the on-site Coulomb interaction. It is very important to mention that in principle, the parameter, *U* is positive because it is a direct Coulomb integral.

In this study, the system described by Equation 1 is one-dimensional, has Periodic Boundary Conditions (PBC) and the number of electrons is equal to the lattice size *L*. The site index in Equation 1 takes values from $1 \leq i \leq L$ with indices 1 and $L+i$ being equivalent. The full Hilbert space for our eight-site ring without applying any symmetry is ($^{16}C_8$) or 12870 states and for the ten-site problem is 184756 states. In order to understand the complex physics of the strongly correlated states, we also plotted the entanglement entropy, *S,* with respect to interaction strength, *U/t*, to reveal the cause of the spin and the charge with different distribution under different conditions along the chain.

Density matrix renormalization group

This aims to give a brief overview of the DMRG method, and to introduce some conventions and notation guiding the DMRG technique as given by Alvarez (2009). The *block* is defined to mean a finite set of sites. Let *C* denote the states of a single site. This set is model dependent. For the Hubbard model, it is given by: $C = \{e,\uparrow,\downarrow, (\uparrow,\downarrow)\}$, where *e* is a formal element that denotes an empty state. For the *t-J* model, it is given by $C = \{e, \uparrow, \downarrow\}$, and for the spin 1/2 Heisenberg model by $C = \{\uparrow,\downarrow\}$. A *real-space-based Hilbert space V* on a block *B* and set *C* is a Hilbert space with basis B^C. This will simply be denoted as *V(B)* and assumed that *C* is implicit and fixed. A *real-space-based Hilbert space* can also be thought of as the external product space of #*B* Hilbert spaces on a site, one for each site in block *B*. We will consider general Hamiltonians that act on Hilbert spaces *V*, as previously defined.

The description of this DMRG technique procedure as given by Alvarez (2009) is as following: the initial system and initial environment are represented by block *S* and *E* respectively as shown in Figure 1. Let us consider two sets of blocks *X* and *Y*. The blocks will be added one at a time from *X* to *S* and from *Y* to *E*. It is of great importance to note that *X* and *Y* are sets of blocks whereas *S* and *E* are basically blocks. All sites in *S*, *X*, *Y* and *E* are numbered. We now start a loop for the DMRG "infinite" algorithm by setting *step* = 0 and *VR (S)* ≡ *V(S)* and *VR (E)* ≡ *V(E)*.

The system is grown by adding the sites in X_{step} to it, and let $S' = S \cup X_{step}$, that is, the *step* th block of *X* to *S* is added to form the block *S'*; likewise, let $E' = E \cup Y_{step}$. Let us form the following product Hilbert spaces: $V(S') = V_R(S) \otimes V(X_{step})$ and $V(E') = V_R(E) \otimes V(Y_{step})$ and their union $V(S') \otimes V(E')$ which is disjoint.

By considering $\hat{H}_{S'\cup E'}$, the Hamiltonian operator, acting on $V(S') \otimes V(E')$. We diagonalize $\hat{H}_{S'\cup E'}$ (using Lanczos technique) to obtain its lowest eigenvector:

$$|\psi\rangle = \sum_{i\epsilon V(S'), j\epsilon V(E')} \psi_{i,j} |i\rangle \otimes |j\rangle, \quad (2)$$

Table 1. Comparison of the ground state energies (E_g/t) for two electrons on two sites as a function of U/t (at t=1) from the DMRG calculations with the exact and variational solution. The comparison shows that the results of DMRG become are more accurate with the exact and variational solutions

Interaction strength (U/t)	Energy (E_g/t)			
	Density Matrix Renormalisation Group (DMRG) (This work)	Exact method (Enaibe, 2003)	Modified Lanczos method (Osafile, 2013)	Variational calculation (Enaibe, 2003)
5.00	-0.7016	-0.7016	-0.7016	-0.7016
4.00	-0.8284	-0.8284	-0.8284	-0.8284
3.00	-1.0000	-1.0000	-1.0000	-1.0000
2.00	-1.2361	-1.2361	-1.2361	-1.2361
1.00	-1.5616	-1.5616	-1.5616	-1.5616
0.00	-2.0000	-2.0000	-2.0000	-2.0000
-1.00	-2.5616	-2.5616	-2.5616	-2.5616
-2.00	-3.2361	-3.2361	-3.2361	-3.2361
-3.00	-4.0000	-4.0000	-4.0000	-4.0000
-4.00	-4.8284	-4.8284	-4.8284	-4.8284
-5.00	-5.7016	-5.7016	-5.7016	-5.7016

where $\{|i\rangle\}$ is a basis of $V(S')$ and $\{|j\rangle\}$ is a basis of $V(E')$.

The density matrices for system are now defined as:

$$(\hat{\rho}S)i,i' = \sum_{j\epsilon V(E')} \psi^*_{i',j}\,\psi_{i,j} \tag{3}$$

in $V(S')$, and environment:

$$(\hat{\rho}E)j,j' = \sum_{j\epsilon V(S')} \psi^*_{i,j'}\,\psi_{i,j} \tag{4}$$

in $V(E')$. We then diagonalize $\hat{\rho}_S$, and obtain its eigenvalues and eigenvectors, $w^S{}_{i,i'}$ in $V(S')$ ordered in decreasing eigenvalue order. We change basis for the operator $H^{S'}$ (and other operators as necessary), as follows:

$$(H^{S'\text{ new basis}})_{i,i'} = (w^S)^{-1}{}_{i,k}\,(H^S)_{k,k'}\,w^S{}_{k',i'} \tag{6}$$

In the same way, we proceed for the environment, diagonalize ρ_E to obtain ordered eigenvectors w^E, and define $(H^{E'\text{new basis}})_{i,i'}$

Let m_S be a fixed number that corresponds to the number of states in $V(S')$ that we want to keep. Consider the first m_S eigenvectors w^S, and let us call the Hilbert space spanned by them, $V_R(S')$, the DMRG-reduced Hilbert space on block S'. If $m_S \geq \#V(S')$ then we keep all eigenvectors and there is effectively no truncation. We truncate the matrices $(H^{S'\text{new basis}})$ (and other operators as necessary) such that they now act on this truncated Hilbert space, $V_R(S')$. We proceed in the same manner for the environment.

Now we increase *step* by 1, set $S \leftarrow S'$, $V_R(S) \leftarrow V_R(S')$, $H_{S'} \leftarrow H_S$, similarly for the environment, and continue with the growth phase of the algorithm.

The sites in the system and environment grow in number as more steps are performed in the case of infinite algorithm. Immediately after this infinite algorithm, a finite algorithm commences in such a way that the environment shrinks at the expense of the system, and the system increases at the expense of the environment. In the case of finite algorithm, the total number of sites remains constant allowing for a formulation of DMRG as a variational method on a basis of matrix product states. The advantage of the DMRG algorithm is that the truncation procedure described above keeps the error bounded and small (assuming $m_S = m_E = m$). At each DMRG step (Chiara et al., 2008), the truncation error $\epsilon_{tr} = \sum_{i>m} \lambda_i$, where λ_i are the eigenvalues of the truncated density matrix ρ_S in decreasing order. The parameter m should be chosen such that ϵ_{tr} remains small (Chiara et al., 2008), say $\epsilon_{tr} < 10^{-6}$. For critical 1-D systems, ϵ_{tr} decays as a function of m with a power law, while for 1-D system away from criticality it decays exponentially. Other studies provide more detailed description of the error introduced by the DMRG truncation in other systems (Hallberg, 2006; Rodriguez-Laguna, 2002; Schollwöck, 2005).

The basis is set up in terms of the occupation number basis using bits pattern available in most programming languages. In our DMRG calculations, we obtained the ground state of chains of length up to 10 sites with open boundary conditions. The hopping integral is set at t = 1 and all energies are measured in units of t. The number of states kept at each iteration of the DMRG calculation varies from site to site, however, five number of sweeps were maintained for all the sites for the calculation to converge. The ITENSOR program was used to run the calculation. Clearly, from the input file above, if t1 and V are set equal to zero, we recover the t-U model which is precisely the Hubbard Hamiltonian (Idiodi et al., 2009).

The program was also tested by comparing the calculated energy with the exact, Lanczos and variational solution for varying values of interaction strength (U/t). Since there is a spin degree of freedom for electrons, one would expect the precision to be much lower than that for the spinless case, for keeping the same number of states. However, the precision is still very high for our problem because of the energy gap at half filling in the alternating Hubbard model. Table 1 shows the accuracy of the DMRG method with other methods.

RESULTS AND DISCUSSION

We present and discuss the results of our calculations in this section. Table 1 shows the comparison of the ground state energies (E_g/t) for two electrons on two sites as a

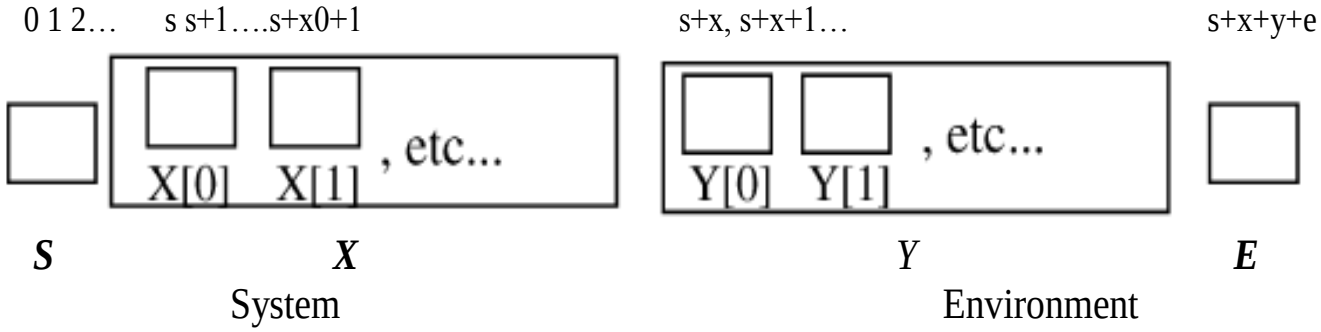


Figure 1. DMRG procedure and blocks labelling. To form the system, the blocks from vector of blocks *X* are added one at a time to block *S* while blocks from vector of blocks *Y* are added one at a time to *E* to form the environment. Blocks are vectors of integers. The numbers at the top of the figure, label all sites in a fixed and unique way (Alvarez 2009).

functions of interaction strength *U/t* values ranging from 5 to -5 (at *t*=1) of the DMRG calculations with the exact and variational solution (Enaibe, 2003) and modified Lanczos (Osafile et al., 2013). It was observed that as the negative values of interaction strength increases, the ground state energy reduces and vice versa in the case of increasing the positive values of interaction strength. It was also observed that at the interaction strength *U/t* = 0, the ground state energy is -2.00 which compared perfectly with the modified Lanczos, exact and variational solution. The comparison shows that the results of DMRG become more accurate with the exact and variational solutions.

The ground state energy dispersion for four electrons on four sites of Figure 2(a) showing the graph of energy versus *t* for various values of *U* (*U* = 0, 1, 2), the hopping term was gradually increased from no hopping (*t* = 0) to maximum hopping (t = 1). It was observed that at any constant value of *U,* the ground state energy reduces as hopping parameter, *t* increases, but at no hopping (*t* = 0), the E_g equals zero at all constant values of *U.* Moreover, our results reveal that for non-interacting *U* =0, there are linear decrease in E_g as *t* increases for all the lattice sites. Figure 2(b) shows the plot of the ground state energy (E_g/t) versus interaction strength (*U/t*). The energy increases linearly initially with the interaction strength and saturates at around E_g/t = -0.25. The result of our calculation is similar to that of exact solution (Onaiwu and Okanigbuan, 2013) as shown in Figure 1(c). Similar results were obtained by Canio and Mario (1996) and Babalola et al. (2011) (Figure 1c).

Figure 3 is the energy dispersion for eight electrons on eight sites. (a) is the energy versus *t* for various values of *U* (*U* = 0, 1, 2, 3), the hopping term was gradually increased from no hopping (*t* = 0) to maximum hopping (*t* = 1) and (b) is the plot of the ground state energy (E_g/t) versus interaction strength (*U/t*). The result of our calculation is similar with that of exact solution (Onaiwu and Okanigbuan, 2013) as shown in Figure 2(c).

Figure 4 shows the plot of ground state energy/t versus *U/t* for ten electrons on ten sites. Figure 4(a) is E_g/t versus t for various values of *U* from *U* = 0, 1, 2 and 3; whereas Figure 4(b) is the variation of the E_g/t with *U/t*.

Figure 5 shows the variation of E_g/t with respect to *U/t* for the indicated values of *N*. We observed generally that with *U/t* = 0, the corresponding value $E_g/t = -N$ for $N \leq 2$.

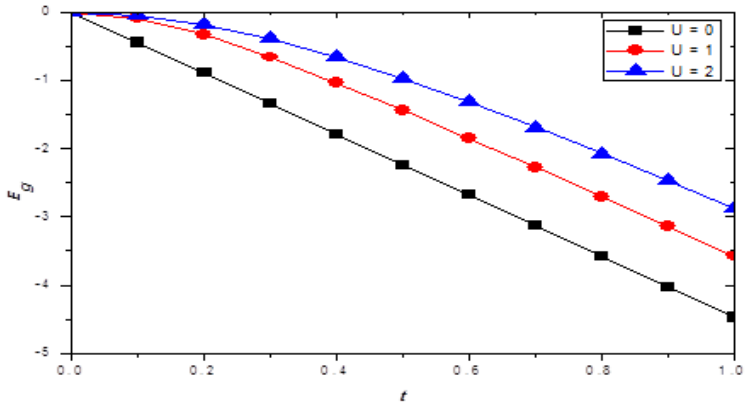
Meanwhile, Figure 6 simply shows the variation of maximum entropy 'S' obtained from the five sweeps of our calculations with respect to interaction strength '*U/t*' for the indicated values of *N*. We then observed a different formation that with *U/t* = 0, the entropy 'S' values are not sequential as in the case of E_g/t versus *U/t* where at *U/t* = 0, the E_g/t decreases as *N* increases as shown in Figure 4. But in the case of maximum *S* versus *U/t*, it does not follow any regular pattern. At *U/t* = 0, *S* = 1.5157 (highest value obtained) for *N* = 10, while the lowest is *S* = 0.8266 at *N* = 4.

Conclusion

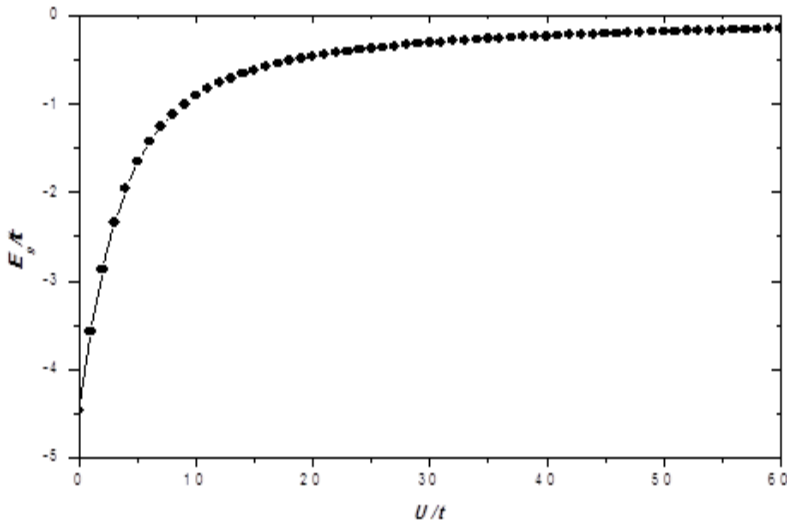
The renormalization group is a powerful technique to determine low energy properties of one-dimension many-body systems. We have successfully applied DMRG to one-dimensional Hubbard model for the number of electrons greater than or equal to two but less than or equal to ten and showed the plot of maximum entropy '*S*' versus interaction strength from two to ten sites (Figure 6) and verified that the ground state energy (E_g/t) decreases as the interaction strength (*U/t*) increases. With low computational cost, this study has shown that the DMRG method is one of the most efficient and versatile algorithm to solve the problem related to strongly correlated electron systems.

It has been shown clearly how versatile and effective the application of DMRG technique to one-dimensional Hubbard model is. The programme successfully tackles larger electrons at half filling. An effort to apply DMRG to two-dimensional Hubbard model has not been successful. Our next study will center on applying DMRG

(a)



(b)



(c)

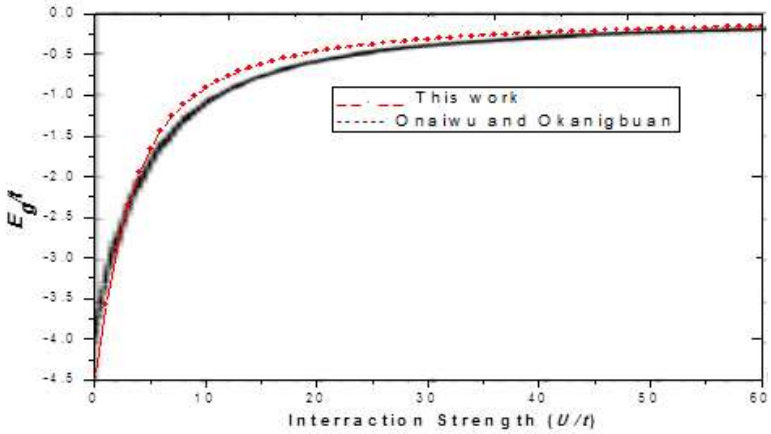
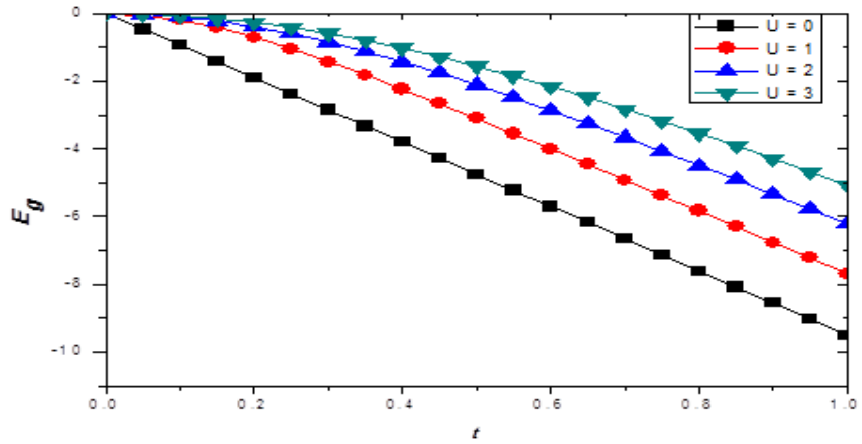


Figure 2. The plot of dispersion curve for four electrons on four sites (a) is the energy (E_g) versus hopping energy (t) at different values of Coulomb interaction (U) as shown in the legend (b) Variation of E_g/t with the on-site energy U/t (c) shows similar result obtained from exact solution by Onaiwu and Okanigbuan (2013).

(a)



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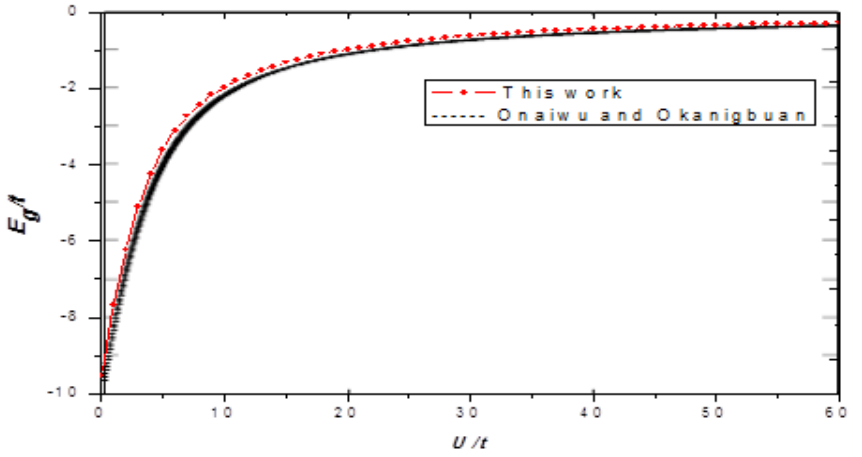
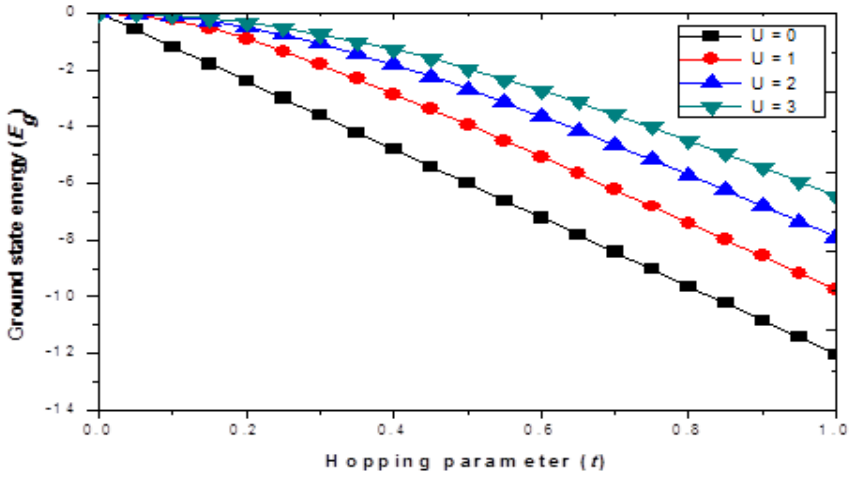


Figure 3. The ground state energy (E_g/t) versus U/t for eight electrons on eight sites. (a) is ground state energy (E_g/t) versus hopping term (t) for various values of U as shown in the legend (b) is the variation of the E_g/t with U/t with good agreement with exact solution by Onaiwu and Okanigbuan (2013).

(a)



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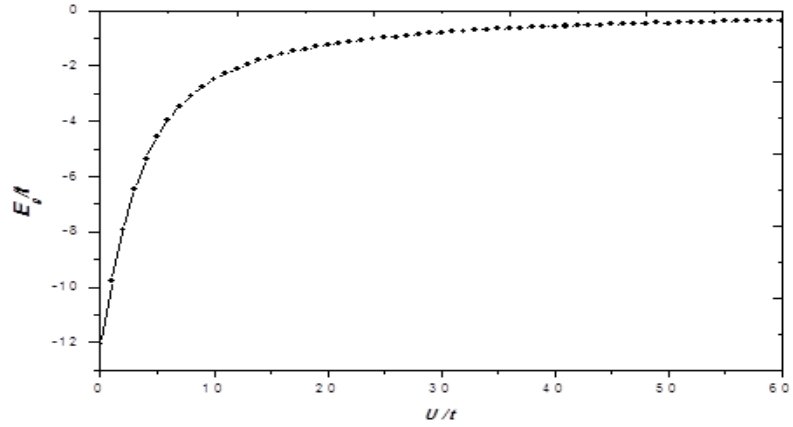

Figure 4. The ground state energy/t versus *U/t* for ten electrons on ten sites. (a) is E_g/t versus *t* for various values of *U* from *U* = 0, 1, 2 and 3 while (b) is the variation of the E_g/t with *U*/tr

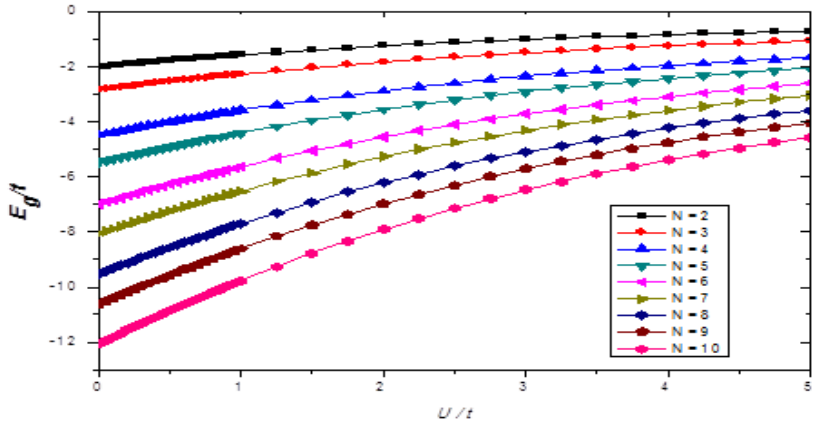

Figure 5. Plot of ground state energy (E_g/t) against interaction strength (*U/t*) for various values of number of electrons *N*.

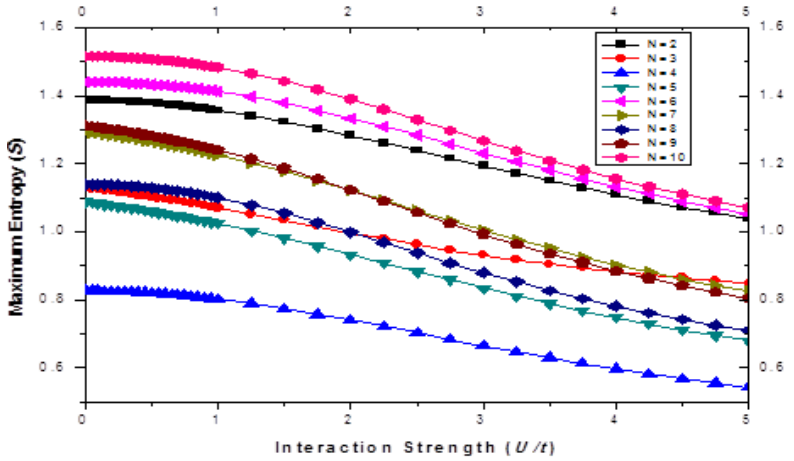

Figure 6. The effect of interaction strength, *U/t*, at *t* = 1 on the energy-dependent entropy, *S*, showing a clear distinction between the attractive and repulsive Hubbard models.

to larger lattice sizes (far more than ten lattices) at half filling and check for how accurate our calculation will be.

CONFLICT OF INTERESTS

The authors have not declared any conflict of interests.

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APPENDIX

Supported file for the work

```
Input
{
N = 2
Npart = 2

t1 = 1
t2 = 0
U = 5
V1 = 0
nsweeps = 5
Sweeps
{
1  Maxm=50, Minm=10,   Cutoff=1.0E-12, Niter=2, Noise=1.0E-07
2  Maxm=100, Minm=20, Cutoff=1.0E-12, Niter=2, Noise=1.0E-08
3  Maxm=200, Minm=20, Cutoff=1.0E-12, Niter=2, Noise=1.0E-10
4  Maxm=400, Minm=20, Cutoff=1.0E-12, Niter=2, Noise=0.0E+00
5  Maxm=800, Minm=20, Cutoff=1.0E-12, Niter=2, Noise=0.0E+00
}
quiet = yes
}
```

Figure S1. The ITensor DMRG input file for single band Hubbard model