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**International Journal of Physical Sciences** 

Review

# Designing off-grid hybrid energy supply with photovoltaics in Senegal

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#### Received 31 August, 2018; Accepted 10 December, 2018

In Africa, electrification of rural areas are low and off-grid power supply is needed. Often diesel generators are used to provide local electricity supply. However, the tremendous decrease in the costs of photovoltaics provides an attractive option to substitute existing diesel generation or to build up a new electricity supply in those locations, lowering power costs and environmental impact. Photovoltaics (PV) hybrid system combines photovoltaics with diesel generators and batteries. The design of PV hybrid systems requires an in-depth analysis of load, solar resources and the interaction between PV, diesel generator and storage for the appropriate sizing of components. The team at CIRE TH Cologne has undertaken several projects to examine the feasibility of such PV hybrid systems in different African locations, e.g. a generic Senegalese village in the Thies region. In addition, a modelling tool was developed to analyze the benefits and optimum setup of PV hybrid systems. Furthermore, hands-on experience was gained by installing a PV hybrid system in Ghana, proving the local benefits of this rather new energy source.

**Key words:** Photovoltaic hybrid system, load profiles, energy system modelling, photovoltaics project planning, installation.

#### INTRODUCTION

In Senegal, like in several other African countries, electrification rates of the rural areas are low and off-grid power supply is needed. In many cases, diesel generators are used to provide electricity supply, more than 1 million diesel generator systems are used worldwide for this purpose. The tremendous decrease in the costs for solar power makes photovoltaics an attractive option to substitute existing diesel generation or to build up a new electricity supply in those locations, lowering power costs and environmental impact. In combination with batteries, photovoltaics may even fully substitute existing diesel generator systems. However, the design of such a system requires an in-depth analysis of load, solar resources, and the interaction PV, diesel generator and storage for the appropriate sizing of the components. However, little is known about the right setup and design needs for such a system.

At CIRE at TH Cologne, a feasibility study for the design of an off-grid power system including photovoltaics, batteries and diesel generator was carried

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Author(s) agree that this article remain permanently open access under the terms of the <u>Creative Commons Attribution</u> <u>License 4.0 International License</u> out for a typical Senegalese village. This feasibility study is based on an extensive literature review of the state of the art of technology and research, the experience from developing numerical simulation tools, the communication with suppliers of components (especially diesel generators, photovoltaics and batteries) and the in planning and installation of comparable projects in Africa and South America. Firstly, the energy needs of a typical Senegalese village were investigated. This required the determination of the load curves with the dedicated free internet tool LoadProGen. Secondly, data on the solar resources was collected. Thirdly, the off-grid hybrid energy supply was modelled with the common software tools PV\*Sol and HOMER to determine the size of the different components. Altogether, this project has yielded valuable insights into the methodological approach, tools, and data available for designing off-grid energy systems. Thus, it is providing results as the basis for real projects in Senegal.

In addition, the results from other projects at TH Cologne in this research field are presented. This includes the creation of a modelling tool to examine the possibilities and limits of integrating photovoltaics into existing diesel generator systems. It considers the setup and operating modes of the diesel generators (with aging and partial load effects), also taking into account the use of batteries (including different types of batteries and aging processes). As a result, the optimum setup of the re-designed hybrid PV-diesel-battery system can be calculated.

Furthermore, the hands-on experience from a recently finished installation of a 90 kW PV hybrid system at the St. Dominic's Hospital in Akwatia/Ghana will be covered. It shows the lessons learned on how such a project could be implemented from the first evaluation of energy data to the final installation on the rooftops.

Altogether, the research hypothesis can be formulated as follows: Given the lack of information, scientific evidence and basic data (e.g. load, solar irradiation), how can a hybrid photovoltaics energy systems be setup properly for a generic village in Senegal and what steps are needed for this, both scientifically and practically?

# GENERAL SETUP AND BENEFITS OF A PV HYBRID SYSTEM

Photovoltaics hybrid systems combine power generation from photovoltaics with diesel generators and batteries. They can be grid-connected to the public electricity grid or operate as island power supplies without a grid connection. As scalable solutions, they can supply a single house with a load below 1 kW up to a commercial premise or hospital with a load of several hundred kilowatts.

The tremendous decrease of the costs for solar power makes photovoltaics an attractive option to substitute

existing diesel generation or to build up a new electricity supply in those locations, lowering power costs and environmental impact (e.g. soot and noise). In combination with batteries, photovoltaics may even fully substitute existing diesel generator systems.

In Senegal, PV hybrid systems can help to improve the rural electricity supply with currently less than 30% electrification rate, increase the share of local renewables (more than 90% of electricity is produced from fossil fuels) and decrease the dependency from energy imports (all fossil fuels are imported).

When setting up a PV hybrid system, the following aspects need to be analysed:

(1) Load patterns: how much electricity is needed by whom (private or commercial consumers) at what time for what purpose (e.g. lighting, cooking, manufacturing)

(2) Renewables resources: which renewables resources are available on the spot (e.g. solar, wind, hydro), in the following only solar resources will be considered

(3) Storage capacities: how much electricity can be stored

(4) Interaction of components: PV, diesel generator and storage interact and depend from each other and have technical boundary limits (e.g. minimum load of generator, ramps of PV with clouds and rain).

#### LOAD PATTERNS AND PROFILE

The load pattern is the basis for the design of the energy system. But how can you estimate the electricity needs of people who have not had any access to it before? To accomplish this, a generic rural village was created based on the findings on a study made on 30 unelectrified rural villages in Senegal. This generic village covers 350 inhabitants in 27 households. The load profile was then created on the basis of the freely accessible platform LoadGenPro as provided by the Politecnico di Milano (Italy) (accessible via Facebook). LoadGenPro has been developed on the basis of extensive research work on typical loads and energy consumption behaviour in Africa and so far provides the most suitable numerical tool for this purpose. The interface of this platform is as shown in Figure 1. It allows to include several electrical appliances and types of consumers.

As a result, the load profile of the generic Senegalese village is as shown in Figure 2. Starting from a rather low consumption at night, the load increases in the morning hours to reach the first peak of 6 kW at 9 h and an afternoon peak of around 7 to 8 kW from 14 h onwards till 22 h (resp. 2 to 10 pm).

However, the experience from commercial projects shows that electricity consumption is not only influenced by the need for light or other electrical appliances but also the willingness, respectively ability of the consumers to pay for power supply. So, load patterns are also

LoadBroCon	Edit configuration					
LoadProgen	User classes	Appliance within class	Appliance details			
POLITECNICO NI ANDITO	Add Rename Delete	Add Rename Delete	Nominal power rate [W]	211		
Save and load	SL 2	Radio A	Functioning cycle [h]	1		
	SL_4 Public lights	B&W TV	Functioning time [h]	3		
Stea current workspace	Public Building Commercial Building		Random variation of func. time [%]	10		
Load on existing undergade	Water Pump		Random variation of func. window [%]	10		
Contracting workspace			Specific cycle not available with this time sample			
'arameters			Functioning windows [h]			
Number of profiles 365			Start End			
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○ 15 min ● 1 h						
oad profiles generation						
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Generate Visualize	within class	for user 5				

Figure 1. Interface of LoadProGen platform to create load profiles (source: LoadProGen by Politecnico di Milano).



Figure 2. Load profile of generic Senegalese village. Source: CIRE/TH Cologne.

influenced e.g. by the time when workers are paid. Furthermore, seasonal or temporal mobility of inhabitants may have influence the overall load.

#### SOLAR RESOURCES IN DIOURBEL REGION

In most locations, renewables resources are limited to

solar irradiation and the space for installing photovoltaics on buildings or ground-mounted. The region of Thies provides a rich average global horizontal irradiation of 2,150 kWh/m<sup>2</sup> in a year (Source: SolarGIS). Figure 3 shows the annual distribution which provides a rather stable daily radiation (left axis) between 5 and 7 kWh/m<sup>2</sup>/day, depending on the clearness index (right axis). This data is usually derived from several years'



**Figure 3.** Load profile of generic Senegalese village. Source: Meteonorm 7.

Table 1. Modelling results for the generic village in Thies region – sizing of components.

Cofficience to al	Architecture					COE
Software tool	Batteries (kW)	Diesel-Gen. (kW)	PV (kW)	Converter (kW)	Type of dispatch	(€/kW)
Homer	5.94	9.20	38.9	9	LF	0.233
PV×Sol	10.65	8.33	19	20	CC	0.25

Source: PV×Sol/Homer applied at CIRE/TH Cologne.

average data, so deviations may occur in individual years. Furthermore, it needs to be mentioned that solar resource data may be hard to investigate or even not available at all for specific African locations.

This distribution of solar irradiation with a rather low spread is a reliable basis for photovoltaics power generation over the entire year, like in many African countries. In contrast, values in Germany have a seasonal spread between 5% (December) and 100% (June) over the year.

#### MODELLING THE PV HYBRID SYSTEM

To find the optimum setup of the PV hybrid system, two different software platforms were used: PV\*Sol and HOMER (PV\*Sol is commercial, while HOMER can be tested for free for a limited amount of time). In this simplified analysis, no care was taken of potential limitations for installing photovoltaics, e.g. limited roof or ground space and shading. Other effects, like efficiency losses due to the warming of the solar cells are taken into account. The modelling was carried out taking into account the load pattern and solar resources. The modelling tools automatically analyzed the setup to provide an optimum setup. However, as shown in Tables 1 and 2, results strongly deviate between the two tools, leading to two totally different setups. However, the costs of energy (COE) are similar, around 0.25 €/kWh.

These deviations are based on the very different setup of the tools, with different approaches on:

(1) The precision of solar irradiation data and calculation of electricity yield from solar irradiation

- (2) Efficiencies of components,
- (3) Dispatch, charging and discharging of batteries

(4) Economics underlying assumptions (e.g. price increases of diesel fuel)

(5) Mathematical logic in the tools and different blocks of it

(6) Costs of operations and maintenance

It needs to be considered that not all information on underlying logic and basic assumptions are made public by the providers.

#### SETUP OF MODELLING TOOL AT TH COLOGNE

Due to the limitations of available numerical modelling tools, the team at TH Cologne developed a MatLab/Simulink based tool for PV hybrid systems. MatLab/Simulink allows using different programming blocks for each technical component which then are

Parameter			Homer	PV×Sol
Consumption	Total per year	[kWh]	35,495	35,495
Consumption	Load peak	[kW]	8.3	8.3
PV array	Production	[kWh/year]	64,821	32,176
Diesel Genset	Production	[kWh/year]	1,124	11,278
	Fuel consumption	[l/year]	393.4	3,591
Battery	Consumption coverage	[kWh/year]	18,456	19,537
Converter	Energy in	[kWh/year]	36,516	35,275
	Energy out	[kWh/year]	34,690	21,176
System	COE	[€/kWh]	0.233	0.25

Table 2. Modelling results for the generic village in Thies region – energy flows.

Source: PV×Sol/Homer applied at TH Cologne.



Figure 4. Setup of PV hybrid modelling tool . Source: CIRE/TH Cologne.

connected via mathematical operations and routines. These "modelling blocks" are as shown in Figure 4. The technical elements PV, diesel generator and load are connected via the energy management which decides on how the electricity is flowing (e.g. from PV to load, but not from a diesel generator to battery). Furthermore, the diesel generator operating modes decide on which diesel generator is operated at which load (if more than one genset is available). The block "PV-system" converts the irradiation into electric power. The block "Battery" includes the parameters of the battery (e.g. state of charge) and the mathematical logics which describe the electrochemical behavior and aging of the battery. "Diesel Generators" cover fuel demand per kWh depending on load factor, a minimum load of the diesel generator and its aging. It is worth noting that partial load puts a greater stress on the diesel generators due to coking and incomplete lubrication. "Output" is a set of calculation results, e.g. costs of energy, charging cycles or optimum setup based on iterative calculations.

It is obvious that this kind of modelling tool is able to

provide more detailed analysis and allows more individual settings (e.g. of interest rates or fuel prices) than the tools described earlier. In Figure 5, the input and output of the modelling tool is listed in more detail. It furthermore shows the results for a specific application case, where a maximum of savings could be found by an optimum combination of PV, batteries and diesel generator. Results also show that due to the spinning reserve of diesel generators (that is, the minimum load possible), it is better to split large diesel generators into smaller units (e.g.  $3 \times 70$  kW instead of  $1 \times 210$  kW, while optimum battery depends on the PV size.

In an ongoing research project at TH Cologne, this modeling tool has been refined to cover a wide range of different diesel generators and provide more flexible and precious modelling.

#### PRACTICAL EXPERIENCE ON-SITE

The CIRE team was also involved in the planning and



Figure 5. Input and output of modelling tool and results from specific analysis. Source: CIRE/TH Cologne.



**Figure 6.** Installation of a photovoltaics hybrid system in Ghana (source: CIRE/TH Cologne)

installation of the "Father Franz Kruse Solar Energy Project" at the St. Dominic's Hospital in Akwatia/Ghana in cooperation with the charity organization "Kindermissionswerk" and "Begeca". This project covered the installation of 90 kW of photovoltaics on different roofs of the Hospital's premises. Frequent power cuts at any time of the day require the use of large diesel generators. Before the project, the hospital had a load between 50 kW at night times and weekends, and up to 160 kW at working days. When grid connected, PV reduces the load taken from the public grid. At times of blackouts, PV reduces the load of the diesel generators. Due to the connection to the public grid, no batteries were included in the setup. In addition, more than 550 LED lights were installed to decrease the electricity demand of the hospital significantly (by more than 20%). It is worth noting that before setting up generating capacities, reducing the electrical demand should be prioritized in such a case.

The measurements after the installation show a significant reduction of electricity consumption form public grid and diesel generation. Besides the fuel and costs savings, the PV Ghana project was a first step for implementing PV in Ghana. Within a few days, local craftsmen were trained to safely and reliably install photovoltaics on the Hospital's premises (Figure 6) and to take care of its operations and maintenance. This proves that photovoltaics cannot only provide a suitable and sound energy source, but also the opportunity for local training, qualification of skilled workers and value

creation.

#### Conclusion

Hybrid energy systems combing renewables (especially solar power from photovoltaics), diesel generators and batteries provide a new alternative source of energy supply in Africa. They can provide new power at off-grid locations and substitute diesel power, providing a with local value creation. The works of the CIRE at TH Cologne in this field proved the feasibility of this concept for a generic village in Senegal. However, modelling tools need to be used carefully due to their different underlying Cheaper and more environmentally sound setups. energy source It allows the optimum setup of PV hybrid systems. In addition, the experience from the "Father Franz Kruse Solar Energy Project", a PV hybrid project planned and installed by the CIRE team vielded valuable practical experience, showed the technical feasibility and proved the local benefits for professional education and qualification. Therefore, PV hybrid systems should play a major role in the future African energy mix and the education of the required technical specialists.

#### **CONFLICT OF INTERESTS**

The authors have not declared any conflict of interests.

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International Journal of Physical Sciences

Full Length Research Paper

# 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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Author(s) agree that this article remain permanently open access under the terms of the <u>Creative Commons Attribution</u> <u>License 4.0 International License</u> 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  $2 \le N \le 10$ . The maximum entropy with respect to interaction strength is also presented.

#### METHODOLOGY

#### Model and parameters

The single band Hubbard Hamiltonian is written as

$$H = -t \sum_{\langle i,j \rangle \sigma} (c_{i\sigma}^+ c_{j\sigma} + h.c) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$
<sup>(1)</sup>

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  $n_{i\sigma} = c_{i\sigma}^+ c_{j\sigma} c_{j\sigma}$  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 onedimensional, 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  $1 \le i \le L$  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  $\widehat{H}_{S'\cup E'}$ , the Hamiltonian operator, acting on  $V(S') \otimes V(E')$ . We diagonalize  $\widehat{H}_{S'\cup E'}$  (using Lanczos technique) to obtain its lowest eigenvector:

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

<b>Table 1.</b> 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 DMF	G
calculations with the exact and variational solution. The comparison shows that the results of DMRG become are more accurate with the	۱e
exact and variational solutions	

	Energy ( <i>E</i> <sub>g</sub> / <i>t</i> )					
strength ( <i>U/t</i> )	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:

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

in V(S'), and environment:

$$(\hat{\rho}E)j,j' = \sum_{j \in V(S')} \psi_{i,j'}^* \psi_{i,j}$$
(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:

$$(H^{S'new basis})_{i,i} = (W^{S'})^{-1}_{i,k} (H^{S'})_{k,k'} W^{S'}_{k,i}$$
(6)

In the same way, we proceed for the environment, diagonalize  $\rho_E$  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  $m_S \ge \#V(S')$  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  $\lambda_i$  are the eigenvalues of the truncated density matrix  $\rho_S$  in decreasing order. The parameter *m* should be chosen such that  $\epsilon_{tr}$  remains small (Chiara et al., 2008), say  $\epsilon_{tr} < 10^{-6}$ . For critical 1-D systems,  $\epsilon_{tr}$  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 ( $E_{q}/t$ ) 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  $E_{\alpha}$  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  $(E_{\alpha}/t)$  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  $N \le 2$ .

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 manybody 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



**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).





**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).





**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 energydependent 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
t^2 = 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

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