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Correcting Factor for more Accurate Strongly Correlated Electron Systems in the Half Filled Band of the Hubbard Model

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Abstract

We exactly calculate the ground state energy of the Hubbard model for four electrons on four sites and compare our results with that obtained in a recent study where a modification of the Lanczos technique was used. We found that the results of that study under estimated the exact diagonalization result by as much as 100.0% at $U/t = 0$ ***and up to*** $\sim$ ***120.6% at*** $U/t = 5.0$.

Keywords: Hubbard model, Lanczos technique, Exactdiagonalization.

1.0 Introduction

In Ref. [1], Osafile et al. argued that their recent simplified modification of the Lanczos technique revealed a clear-cut formula for obtaining improved ground state energy and wave function of the Hubbard model at every step of iteration.

Here we present the exact diagonalization results for the same four electrons on four sites in order to corroborate or otherwise the claim in [1] that their result for the four-site problem was better than that previously obtained in Ref. [2]. We will also compare our results with those of Ref. [1] and subsequently try to modify their result.

2.0 Method

The Hubbard Hamiltonian is of the form:

$$H = -t \sum_{\langle i,j \rangle \sigma} (C_{i\sigma}^{\dagger} C_{j\sigma} + C_{j\sigma}^{\dagger} C_{i\sigma}) + U \sum_{i} n_{i\sigma} n_{i\sigma'} \qquad (1)$$

where the first term accounts for the hopping of electrons from site to site, t is the hopping parameter, $C_{i\sigma}^{\dagger}(C_{i\sigma})$creates (annihilates) an electron with spin σin the Wannier state localized at lattice site$i$, $\langle \, .. \rangle$ denotes nearest neighbours sites only, σ is the electronic spin, U isthe on-site energy and $n_{i\sigma} = C_{i\sigma}^{\dagger} C_{i\sigma}$ counts the number of particles at site i with spin σ. In this paper, the system described by Eq (1) is one-dimensional, has periodic boundary conditions (PBC) and the number of electrons N is equal to the lattice size L. The site index in Eq (1) takes values from $1 \leq i \leq L$, with indices 1 and $L + 1$ being equivalent.

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The full Hilbert space for a four-site ring without applying any symmetry is $\binom{8}{4}$or 70 states, for eight-site ring without applying any symmetry is $\binom{16}{8}$ or 12870 states and for the ten-site problem it is 184756 states resulting in matrices of 1.6564 $\times 10^8$ and 3.4135×10^{10} entries respectively. Interestingly, these matrices are very sparse. We here present the result for the four- site problem. For a full discussion of the method we employed and the result for other problems, we refer the reader to Ref. [3].

3.0 Results and discussion

First, we determine exactly [3] the ground state energy per unit interaction strength, E_g/t, for four electrons on four sites in the positive on-site energy per unit t, U/t, region. Fig. 1 shows the variation of E_g/t with U/t as compared with previous result [4]. The open circles are our results while the open triangles are those of Ref. [4]. We observe that our results agree greatly with those obtained by Canio and Manio [4].

Fig. 2 is a comparison of our results with those of Ref. [1], the circles are our results and the solid squares are those of Ref. [1]. It can be seen clearly that the result of [1] does not in any way agree with ours. We observe that there is strong disparity between our result and theirs both in the positive and negative U/t values. Worse is the fact the Ref. [1] gives a value far lower than -4.00 at $U/t=0$, an indication that the results/method needs some modifications.

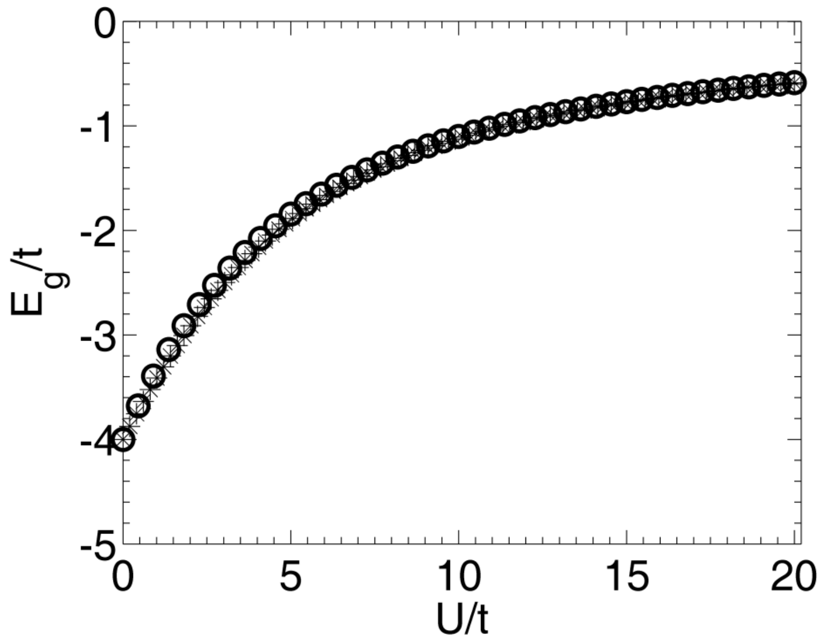

Fig.1The exact diagonalization results of Refs. [3, 4], the open circles are the results of Ref. [3] while the asterisks are those of Ref. [4]. The two results are in perfect agreement in the positive U/t region, as expected. $\boldsymbol{Eg/t = -4}$ when $\boldsymbol{U/t = 0}$ and it approaches zero in the large $\boldsymbol{U/t}$ limit.

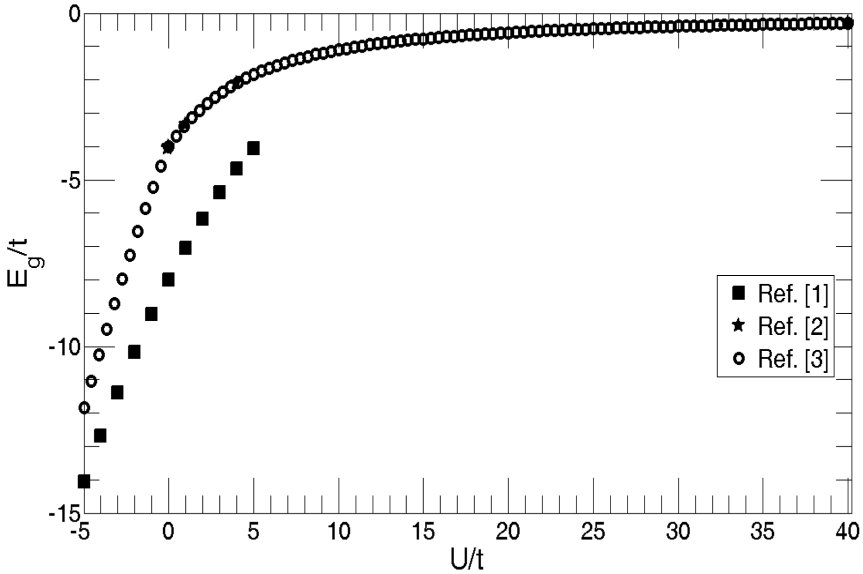

Fig. 2 A comparison of the results ofRefs. [1 − 3]; the solid squares are those of Ref. [1], solid pentagons are the variational calculation results of Ref. [2] while the open circles are the results of Ref. [3]. Observe the strong disparity between the results both in the positive and negative U/t values. Worse is the fact the Ref. [1] gives a value far lower than -4.00 at $U/t=0$, an indication that the results/method needs some modifications.

A close analysis of the result obtained by Ref. [1] as shown in Fig. 2 indicates that the ground state energy was under estimated by as much as 100.0% at $U/t=0$ and up to ~ 120.6% at $U/t=5.0$. The variational calculation results of Ref. [2] are in good agreement with the exact calculation results of Ref. [3, 4]. Due to this observed disagreement with the exact diagonalization results, we say that for the approximation method of Ref. [1] to be taken as a good modification to the Lanczos algorithm there is the need for further modification of the method if it is to properly capture the physics for larger lattice sizes. In view of this, we multiplied the data set by 0.45 and obtained Fig. 3. Clearly, the results became equivalent to exact result when $U/t\geq2.5$ but became higher at lower values of *U/ t*. The claim in Ref. [1] that their result was better than those of Ref. [2] is actually questionable.

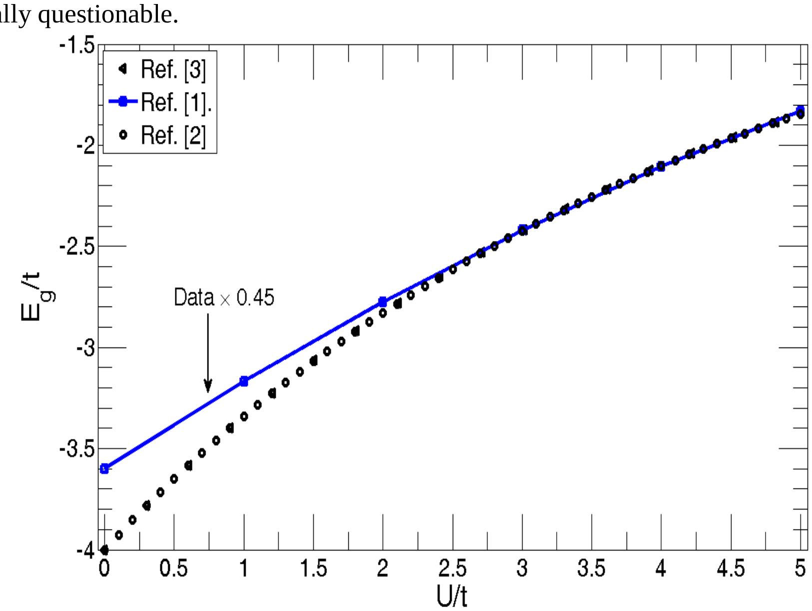

Fig. 3 Plot of the modified data of Ref. [1], when each datum is multiplied by 0.45, the modified data became equal to those of Refs. [2, 3] when $U/t\geq2.5$ but now overshoot their exact counterpart at lower values.

4.0 Conclusion

From the preceding sections, we have been able to obtain a correction to the result of Osafile et al. [1] by multiplying their data by 0.45. This modification made their result agree with the exact diagonalization results of Refs. [2−4] in the region of $U/t \geq 2.5$. A further modification may be required for it to agree totally in the region $U/t < 2.5.$ As the result of Osafile et al. did not go beyond $U/t > 5,$ we could not ascertain how our modification will affect their result in the large U/t limit. In view of the foregoing, we conclude that the claim by Ref. [1] that their result was better than those of Ref. [2] is actually an exaggeration.

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