

Exact Diagonalization of the Hubbard Model: Ten-electrons on Ten-sites

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Abstract: By exactly diagonalizing the Hubbard model for ten electrons on ten sites in a one-Dimensional (1D) ring, we extend the study of Jafari (2008) to more than two electrons on two sites. We equally show the sparsity patterns of the Hamiltonian matrices for four- and eight-site problems and obtain the ground state energy eigenvalues for ten electrons on ten-sites. The technique we employ will be a good guide to a beginner/programmer.

Keywords: Exact-diagonalization, hamiltonian, hubbard model, sparse matrix, spin flip

INTRODUCTION

The Hubbard model (Hubbard, 1963) has been the basic formalism for treating the electron-electron correlations in interacting many-body systems ever since the advent of high- T_C superconductors. 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.

Exact Diagonalization (ED) technique is unique among the various numerical techniques available because it is unbiased, simple and straightforward. However, it is not usually a method of choice because of the high cost of computer memory usage involved (Weiße and Fehske, 2008) except some symmetries are applied which lead to a reduction of the Hilbert space. Jafari (2008) provides some analytic solution for the case of two electrons on two sites. We shall in the subsequent sections extend the study of Jafari to more than two electrons on two sites.

By exactly diagonalizing the Hubbard model, using some intrinsic routines in MATLAB® (R2010a), we present the ground state energy for N electrons on N sites with $4 \leq N \leq 10$. The sparsity pattern of the Hamiltonian matrix is also presented.

METHODOLOGY

The model Hamiltonian is of the form:

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

where,

t : The hopping term

$C_{i\sigma}^\dagger (C_{i\sigma})$: Creates (annihilates) an electron with spin σ in the Wannier state localized at lattice site i
 $\langle .. \rangle$: Nearest neighbors sites only
 σ : The electronic spin
 U : The on-site energy
 $n_{i\sigma} = C_{i\sigma}^\dagger C_{i\sigma}$: Counts the number of particles at site i with spin σ

In this study, 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 $i \leq i \leq L$, 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 resulting in matrices of 1.6564×10^8 and 3.4135×10^{10} entries respectively. Interestingly, these matrices are very sparse.

Exact diagonalization: The basis is set up in terms of the occupation number basis using bits pattern available in most programming languages. The most unsophisticated way of doing this is to write down a piece of code with N loops (Cameron, 1994), which in MATLAB (R2010a) looks like:

```
for i1 = 0 : 2*N-8
    for i2 = i1+1 : 2*N-7
        for i3 = i2+1 : 2*N-6
            :
            for i8 = i7+1 : 2*N-1
                k = 1;
                basis_states (k) = 2^i1 + 2^i2 + 2^i3 + ...
                    + 2^i8;
                (2)
                k = k + 1;
            end
        end
    end
end
:
```

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end
end
end

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The basis_states generated by the code above is sorted in an ascending order, by calling MATLAB intrinsic function sort, for easy referencing. The sorted states are converted into unsigned integer and separated into the spin up and spin down parts; this is necessary since the Hamiltonian Eq. (1) does not mix the up and down spin states. Assuming the numbering of the sites is from the right and that the spin up sites are the first N sites, the separation of the states is easily done with commands:

$$Iup(k) = \text{mod}(\text{basis_states}, 2^N) \quad (3)$$

$$Idwn(k) = \text{basis_states} / 2^N \quad (4)$$

where Iup (Idwn) are respectively the spin up (down) parts.

The Hamiltonian matrix can now be easily set up with the bit manipulation functions, like the bitget (A, bit) which returns the value of the bit at position bit in A; bit must be integer between 1 and 8 unlike FORTRAN where it is from 0 and bitxor (A, B) which returns the bitwise XOR of arguments A and B. Suppose the state Iup (296) is represented by the integer

187 or the binary 10111011, bitget (Iup (296), 3) returns 0; since counting from the right, site 3 is empty. To flip the spins of the electrons at sites I and J, the command bitxor (Iup (k), 2^(I-1) + 2^(J-1)) does it. In other words:

$$C_{i\sigma}^\dagger C_{j\sigma} = \text{bitxor}(Iup(k), 2^{(I-1)} + 2^{(J-1)}) \quad (5)$$

The new state just obtained after the flip operation is recombined with its Idwn (k) counterpart. In particular, if the basis_states (296) (= 110010111011) was split into Iup (296) and Idwn (296), the Idwn (296) counterpart of Iup (296) is 1100 (or integer 12). The new configuration, 10111101 after the spin flip operation bitxor (Iup (296), 2⁽¹⁾ + 2⁽²⁾), can be recombined with the Idwn (k) using the command Idwn (k) * 2^N + bitxor (Iup (k), 2^(I-1) + 2^(J-1)) to obtain basis (jj). This new state, say basis (jj), is checked up using the intrinsic function ismember:

$$[\sim, ind] = \text{ismember}(\text{basis}(jj), \text{basis_states}(k)) \quad (6)$$

in basis_states (k) and the corresponding index, ind, forms the matrix element $T(ind, k) = \pm t$. $T(ind, k) = +t$ only whenever an electron is wrapped around the boundary and the number of electrons it commutes is odd (Weiße and Fehske, 2008). To minimize the

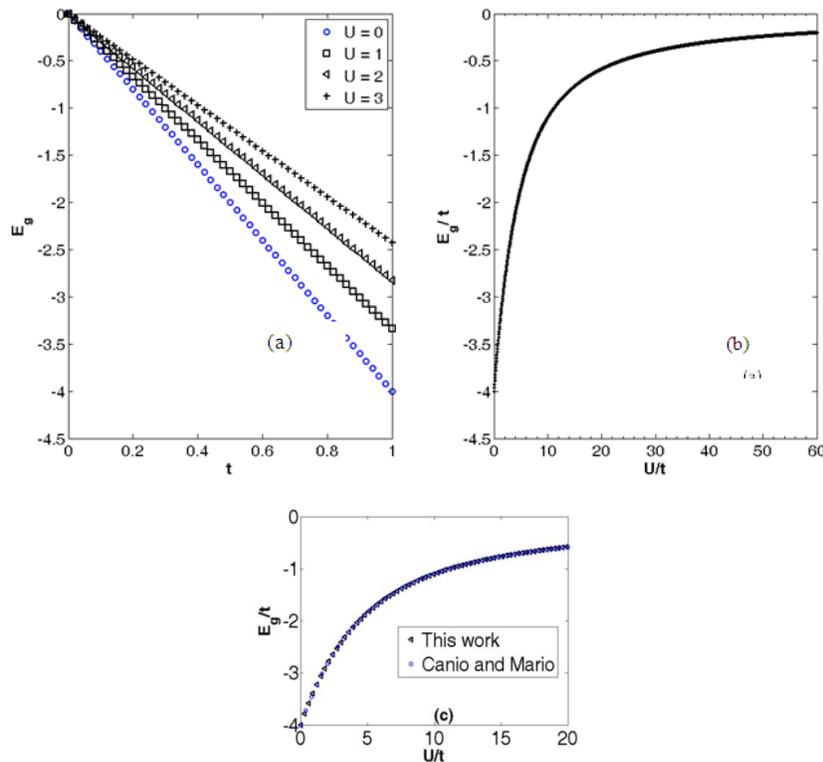


Fig. 1: The plot the dispersion curve for four electrons on four sites, (a) is the energy versus t for the different values of U shown in the legend, (b) is the variation of E_g/t with the on-site energy U/t . Similar result was obtained by Canio and Mario (1996), (Fig. 1c)

computer memory usage, the matrix T should be initially declared as sparse ($T = \text{spalloc}(\text{Ind}, \text{Ind}, N)$). The above description is repeated for the $\text{Idwn}(k)$ states.

The diagonal matrix elements H_{ii} is easy to implement as this is just a matter of counting the doubly occupied sites in both $\text{Iup}(k)$ and $\text{Idwn}(k)$.

Having obtained the matrix H_{ij} , the eigen values are easily obtained using the sparse eigenvalues routine *eigs* in MATLAB; *eigs*($H, n, 'sa'$) returns the n -lowest eigen values of H . The results of our simulations for $N = 3, 4, \dots, 10$ will be presented in the next section.

RESULTS AND DISCUSSION

In this section, we present and discuss the results of our calculations. Figure 1 is the energy dispersion for four electrons on four 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 U/t . Our result agrees with that obtained by Canio and Mario (1996), (Fig. 1c) and at $U/t = 0$, $E_g/t = -4$ was also obtained by Babalola *et al.* (2011) and Edison and Idioidi (2004). Figure 2 shows the sparsity pattern of the Hamiltonian matrix for four electrons on four sites with particles number conservation neglected: the nonzero (nz) entries

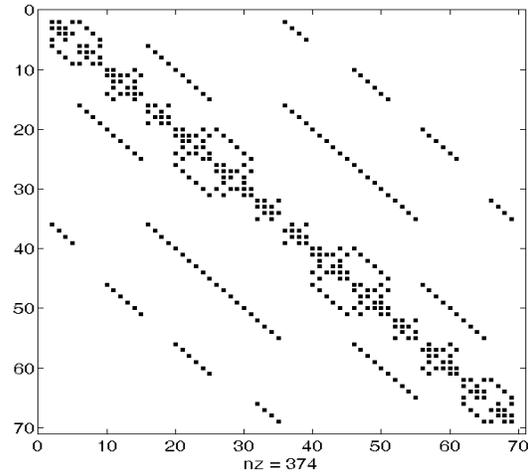


Fig. 2: The sparse matrix of the hamiltonian for four electrons on four sites. Observe that the matrix is actually sparse with only 374 non-zero entries. No symmetry other than PBC is applied

are just 374. So, the matrix is not so large that all the eigenvalues cannot be calculated as stated by Babalola *et al.* (2011). If symmetry operations are even applied, the Hamiltonian acquires a block structure (Weißé and Fehske, 2008).

Figure 3 shows the ground state energy/ t versus U/t for eight electrons on eight sites. The first of the figures

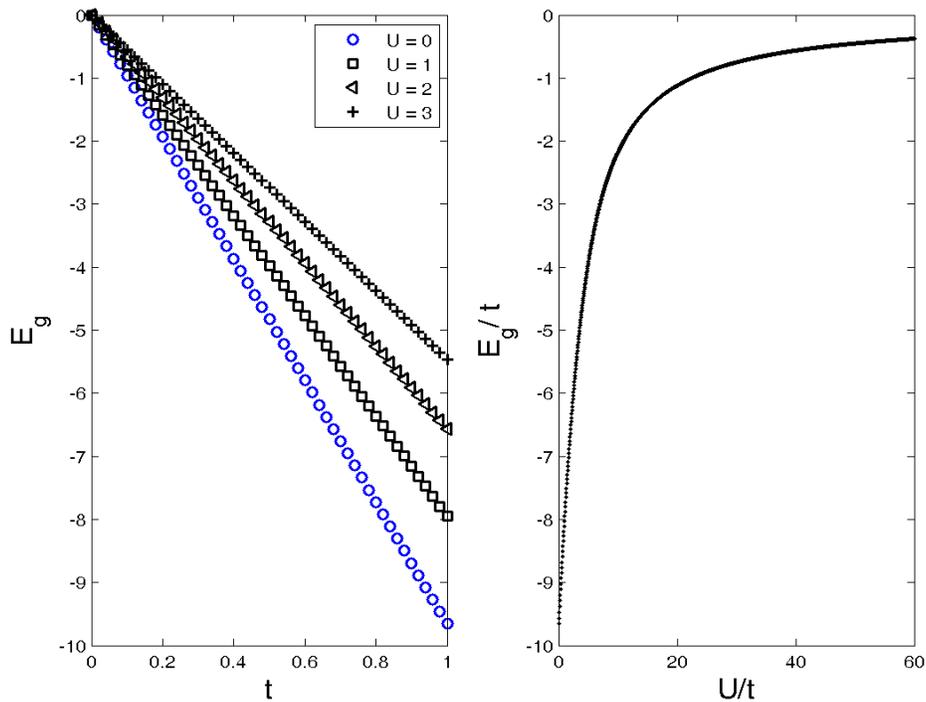


Fig. 3: The ground state energy/ t versus U/t for eight electrons on eight sites. The first of the figures is E_g/t versus t for various values of U from $U = 0, 1, 2, 3$ and the second is the variation of the E_g/t with U/t . Observe that the $E_g/t(0) \neq -8.00$ as was the case for $N \leq 4$ when $E_g/t(0) = -N$

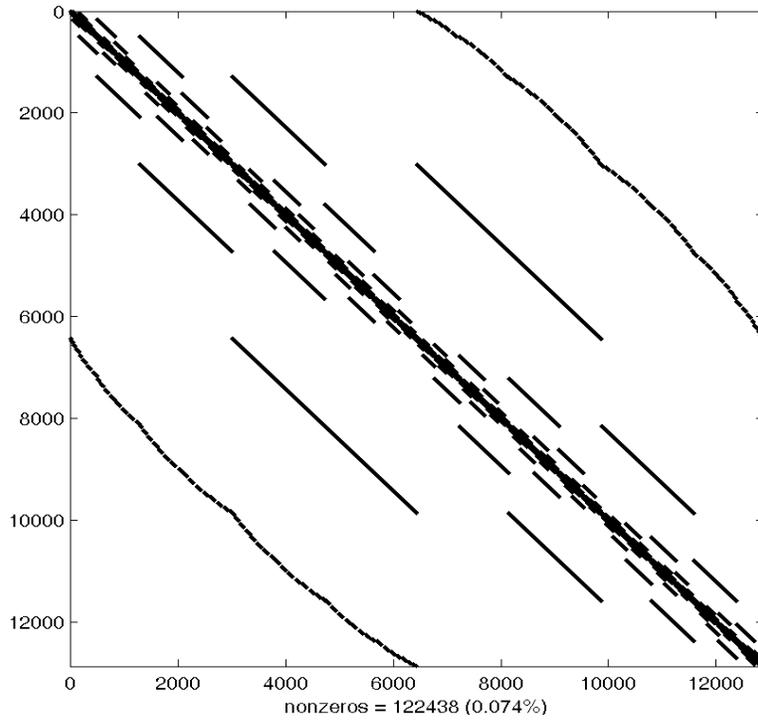


Fig. 4: The sparsity pattern of the hamiltonian matrix for eight electrons on eight sites when particles number conservation is neglected. Observe that only 122438, 0.074%, entries are non-zeros

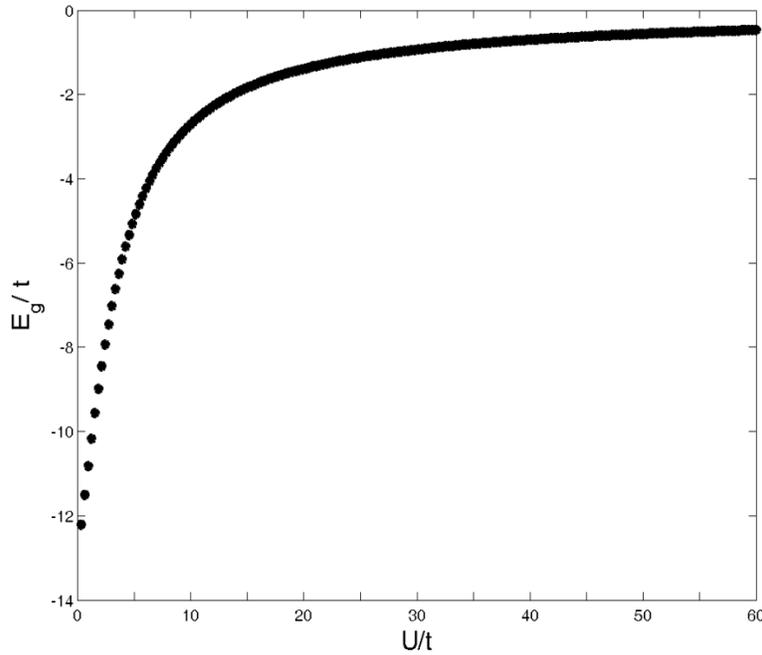


Fig. 5: The variation of the ground state energy with the on-site potential for ten electrons on ten sites; we observed that the ground state energy at $U/t = 0$ is -12.9443

is E_g/t versus t for various values of U from $U = 0, 1, 2, 3$; and the second is the variation of the E_g/t with U/t . We observed that the $E_g/t(0) \neq -8.00$ as was the case for $N \leq 4$ when $E_g/t(0) = -N$.

The sparsity pattern of the Hamiltonian matrix for eight electrons on eight sites when particles number conservation is neglected is shown in Fig. 4. Observe that only 122438, or 0.074%, of the entries are non-

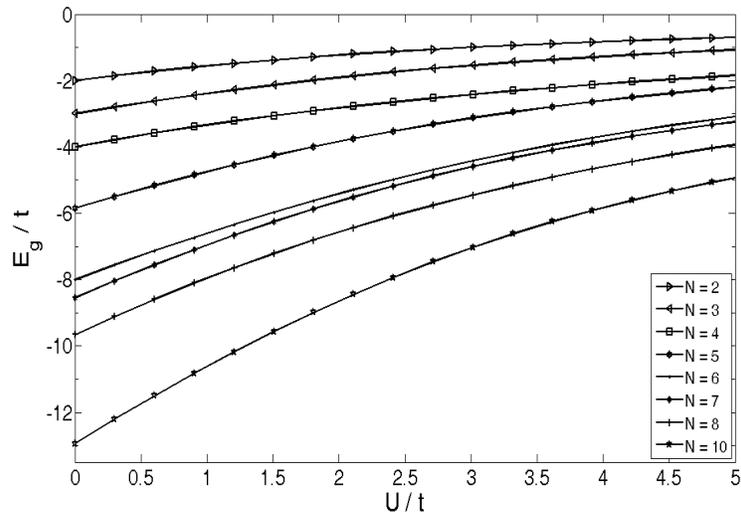


Fig. 6: Plot of E_g/t against U/t for various values of number of electrons N

zeros. Nevertheless, were the states constructed and labeled with a conserved quantum number, the matrix would have broken up into blocks that can be diagonalized separately.

For the case of ten electrons on ten sites, we obtained the graph shown in Fig. 5.

The sparsity pattern of the Hamiltonian matrix for our ten electrons on ten sites problem showed that only 2128532 entries or 0.0062% are non-zeroes.

Figure 6 shows the variation of E_g/t with respect to U/t for the indicated values of N . We observed that with $U = 0$, $E_g/t = -N$ for $N \leq 4$. However, $E_g/t < -N$ for $N > 4$.

CONCLUSION

We have exactly diagonalized the Hubbard model for the number of electrons greater than or equal to four but less than or equal to ten and showed the sparsity pattern of the Hamiltonian matrix when no particles number conservation is applied. We have been able to show that the use of the sparse allocation of the Hamiltonian matrix helped reduce the computer memory usage.

An attempt to modify our program to tackle more than ten electrons at half-filling without applying any symmetry operations was unsuccessful with our low memory personal computer. We intend extending this to take care of more than ten-electron sites by applying appropriate symmetry operations that would not make

the code hard-wired to a particular problem in our next study.

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