Comlexity of the "Strongly Correlated Electrons Model" Problem

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Here goes the abstract....

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I. DEFINITION OF THE PROBLEM

A. Introduction

Let the input size of the problem be N, which will be interpreted as the number of sites. We want to put N_e electrons on these sites in all possible ways. The electrons can have $F = 2$ flavors, that we will call up and down. Also the electrons are indistinguishable, so the order does not matter. No more than one electron of the *same* flavor may occupy the same site (this is called Pauli exclusion principle). We have $\sum_{N_\uparrow=0}^{N_e} C_{N_\uparrow}^N C_{N_e-N\uparrow}^N$ ways of putting these electrons on the N sites. For example, for $N = 4$ and $N_e = 4$ there are $1^2 + 4^2 + 6^2 + 4^2 + 1^2 = 70$ possibilities. The 36 possibilities with 2 electrons up and 2 electrons down, i.e., with $N_\uparrow = N_\downarrow = 2$, are schematically represented in Table. I. To represent these states we use the following notation: a given site can contain (i) no electrons and then it has the number 0, (ii) 1 electron with flavor up and then it has the number 1, (iii) 1 electron with flavor down and then it has the number 2 or (iv) 2 electrons one with flavor up and one with flavor down, and then it will have the number 3. For example, for the state $|3, 2, 1, 0\rangle$, the comma-separated list of numbers gives the electron content of each site, for site 0 to site 3. The first number (3) is for site 0 and the number 3 there means there are two electrons with each flavor. The second number (2) is for site 1 and the number 2 there means that there is an electron with flavor down. The third number (1) is for site 2 and the number 1 there means an electron with flavor or spin up. The last number (0) is for site 3 and the number 0 there means no electrons there.

With these states we form a linear space over the complex numbers by considering a formal sum and multiplication by scalar (complex number). We moreover define a inner product $\langle x_i, x_j\rangle = \delta_{i,j}$ for these states. We call this linear space with inner product the *Hilbert space* for this problem. We will denote this linear space by $\mathcal{V}(N, N_e)$, or simply $\mathcal{V}$ if N and N_e are understood. For example, for $N = 4$ and $N_e = 4$ we have a basis with 70 states, 36 of which are shown in Table. I. A state of the Hilbert space is any linear combination (over the complex numbers) of these 70 states. Once the Hilbert space is defined it will have many bases. Therefore, we introduce here a name for the basis that we used to define it: the *computational basis* or natural basis. Remember that the computational basis is given by elements that are generated by all possible ways of putting N_e electrons on N sites given the constraint that no more than one electron of the *same* flavor can occupy the same site (this is called Pauli exclusion principle).

3,3,0,0	3,2,1,0	3,2,0,1	2,3,1,0	2,3,0,1	2,2,1,1
3,1,2,0	3,0,3,0	3,0,2,1	2,1,3,0	2,1,2,1	2,0,3,1
3,1,0,1	3,0,1,2	3,0,0,2	2,1,1,2	2,1,0,3	2,0,1,3
1,3,2,0	1,2,3,0	1,2,2,1	0,3,3,0	0,3,2,1	0,2,3,1
1,3,0,2	1,2,1,2	1,2,0,3	0,3,1,2	0,3,0,3	0,2,1,3
1,1,1,1	1,0,3,2	1,0,2,3	0,1,3,2	0,1,2,3	0,0,3,3

TABLE I: States for $N = 4$ and $N_e = 4$ that have $N_\uparrow = N_\downarrow = 2$. 0 means no electron at that site, 1 means electron with spin up, 2 means electron with spin down and 3 means two electrons one with spin up and the other with spin down.

Now we will consider a Hamiltonian operator, $\hat{H} : \mathcal{V} \to \mathcal{V}$, acting on this space. We will keep the problem tied to a specific Hamiltonian: the Hamiltonian of the Hubbard model. Let t be a $N \times N$ real symmetric matrix with all diagonal elements equal to 0, and let $U \geq 0$ be a real number. To define $\hat{H}$ we only need to define how it acts on elements of a basis of $\mathcal{V}$. We will do so for the computational basis. We split $\hat{H}$ in two parts:

$$\hat{H} = \sum_{i=0,j=0}^{i<N,j<N} (\hat{K}_{i,j}^{\uparrow} + \hat{K}_{i,j}^{\downarrow}) + \sum_{i=0}^{i<N} \hat{H}_i^{\text{interaction}}. \quad (1)$$

First, for each $|v\rangle$ of the real-space basis, we define the interaction $\hat{H}_i^{\text{interaction}}|v\rangle = x_i U|v\rangle$, i.e. the interaction is diagonal and x_i is 0 if there are less than two electron on site i in vector $|v\rangle$ and 1 otherwise. Second, for each $|v\rangle$ of the real-space basis, we define $\hat{K}_{i,j}^{\uparrow} v\rangle = t_{i,j} s|w\rangle$ such that (i) if $i \neq j$ *and* $|v\rangle$ has an electron with spin up on site j *and* no electron with spin up on site i, then $|w\rangle$ is the vector formed from $|v\rangle$ by moving the electron with spin up on site j to site i *or* (ii) if the condition in (i) before does not hold then $|w\rangle = \emptyset$. In the expression above $s = (-1)^{N_e(i,j)}$, where $N_e(i, j)$ is the number of electrons for all sites from i to j, including i but excluding j, in state $|v\rangle$. This is called the *fermionic sign*. Similarly, we define $\hat{K}_{i,j}^{\downarrow}$ on elements of the real space basis by substituting the previous definition where it says "spin up" with "spin down".

Now we are ready to formulate the problem. We will call this first problem, the *ground state problem*, or *gs problem*: Find the lowest eigenvalue of $\hat{H}$ and corresponding eigenvector.

Is this problem P, NP, NP-complete, QMA, QMA-complete? Before studying this question, though, we need to formalize this section.

B. Compact Notation

Definition 1 States of one site: *Let* $C = \{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$ *be the states of one site. These have the meaning of empty state, up electron, down electron and double occupied as explained before. We will treat this set as formal elements, but we will assume that there is an implicit mapping to the natural numbers 0,1,2 and 3 as indicated.*

Definition 2 Real space state*: Given* $N > 0$*, a real space state is an element of the set* C^N*. There are* $(\#C)^N$ *of these states. We can represent them as* $\bigotimes_i |x_i\rangle$ *where* $|x_i\rangle \in C$*, and* $0 \leq i < N$*.*

Definition 3 Number of electrons of a state*: Let* $\mathcal{N} : C^N \to \mathbb{N}$ *such that* $\mathcal{N} \bigotimes_i |x_i\rangle = \sum_i n(x_i)$*, where* $n(|0\rangle) = 0$*,* $n(|1\rangle) = n(|2\rangle) = 1$*, and* $n(|3\rangle) = 2$*.*

Definition 4 States with fixed number of electrons*: Given* $N_e \geq 0$ *it is the set* $\{|x\rangle \in C^N; \mathcal{N}|x\rangle = N_e\}$

Definition 5 Hilbert space*: For fixed* $N > 0$ *and* $N_e \geq 0$*, it is the linear sub-space over complex number with basis* $\{|x\rangle \in C^N; \mathcal{N}|x\rangle = N_e\}$*, with formal sum and multiplication by a scalar (complex), and moreover endowed by the inner product* $\langle x_i, x_j\rangle = \delta_{i,j}$*. These states with fixed number of electrons are called the real-space basis. The Hilbert space will be denoted by* $\mathcal{V}(N, N_e)$*, or simply by* $\mathcal{V}$*. We will denote like this:* $\emptyset$*, the zero of this space. Do not confuse* $\emptyset$ *with* $|0, 0, 0 \cdots, 0\rangle$*, the state without electrons.*

Definition 6 Number of electrons between two sites *Let* $0 \leq i < j < N$*, then we define* $N_{i,j} : C^N \to \mathbb{N}$ *such that* $N_{i,j} \bigotimes_r |x_r\rangle = \sum_{r=i}^{r<j} n(x_r)$*, where* n *was defined in 3 above.*

Definition 7 Model Parameters *We define* t *to be a real symmetric* $N \times N$ *matrix, and* $U \geq 0$ *a real number.*

Definition 8 Bitwise & **Operator***: We define* $\& : C \times C \to \mathbb{N}$ *such that* & *is a bitwise "and" operator. We assume that the elements of* C *are mapped to the natural numbers 0,1,2,3 as shown in Definition 1*

Definition 9 Bitwise $\wedge$ **Operator***: We define* $\wedge : C \times C \to \mathbb{N}$ *such that* $\wedge$ *is a bitwise "or" operator. We assume that the elements of* C *are mapped to the natural numbers 0,1,2,3 as shown in Definition 1*

Definition 10 Bitwise $\rhd$ **Operator***: We define* $\rhd : C \times \{1\} \to \mathbb{N}$ *such that* $\rhd$ *is a bitwise "rightshift" operator. We assume that the elements of* C *are mapped to the natural numbers 0,1,2,3 as shown in Definition 1. For example* $1 \rhd 1 = 0$*,* $2 \rhd 1 = 1$*,* $3 \rhd 1 = 1$*, etc.*

Definition 11 Kinetic Energy Operator $\hat{K}^{\uparrow}$*:* $\hat{K}^{\uparrow}_{i,j} : \mathcal{V} \to \mathcal{V}$*, is given by (i) if* $x_i \& 1 = 0$ *and* $x_j \& 1 \neq 0$ *then* $\hat{K}^{\uparrow}_{i,j} \bigotimes_r |x_r\rangle = t_{i,j} s_{i,j} \bigotimes_r |y_r\rangle$*, where* $y_r = x_r$ *if* $r \neq i$ *and* $r \neq j$*,* $y_j = x_j \& 2$ *and* $y_i = x_i \wedge 1$*,* $s_{i,j} = (-1)^{\hat{N}_{i,j} \bigotimes_r |x_r\rangle}$ *and (ii)* $\emptyset$ *otherwise. Note that* $\hat{N}_{i,j} \bigotimes_r |x_r\rangle$ *is a natural number according to Definition 6.*

Definition 12 Kinetic Energy Operator $\hat{K}^{\downarrow}$*:* $\hat{K}^{\downarrow}_{i,j} : \mathcal{V} \to \mathcal{V}$*, is given by (i) if* $x_i \& 2 = 0$ *and* $x_j \& 2 \neq 0$ *then* $\hat{K}^{\downarrow}_{i,j} \bigotimes_r |x_r\rangle = t_{i,j} s_{i,j} \bigotimes_r |y_r\rangle$*, where* $y_r = x_r$ *if* $r \neq i$ *and* $r \neq j$*,* $y_j = x_j \& 1$ *and* $y_i = x_i \wedge 2$*,* $s_{i,j} = (-1)^{\hat{N}_{i,j} \bigotimes_r |x_r\rangle}$ *and (ii)* $\emptyset$ *otherwise. Note that* $\hat{N}_{i,j} \bigotimes_r |x_r\rangle$ *is a natural number according to Definition 6.*

Definition 13 $\hat{n}_{i\uparrow}$ **Operator***:* $\hat{n}_{i\uparrow} : \mathcal{V} \to \mathcal{V}$*, is given by*

$$\hat{n}_{i\uparrow} \bigotimes_r |x_r\rangle = (\sum_s (x_s \& 1)) \bigotimes_r |x_r\rangle. \tag{2}$$

Note that this gives the number of electrons with spin up at site i*.*

Definition 14 $\hat{n}_{i\downarrow}$ **Operator***:* $\hat{n}_{i\downarrow} : \mathcal{V} \to \mathcal{V}$*, is given by*

$$\hat{n}_{i\downarrow} \bigotimes_r |x_r\rangle = (\sum_s (x_s \& 2) \rhd 1) \bigotimes_r |x_r\rangle. \tag{3}$$

Note that this gives the number of electrons with spin down at site i*.*

Definition 15 $\hat{H}$ **Operator***: The Hamiltonian operator* $\hat{H} : \mathcal{V} \to \mathcal{V}$ *is given by*

$$\hat{H} = \sum_{i,j} (\hat{K}^{\uparrow} + \hat{K}^{\downarrow}) + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} \tag{4}$$

Definition 16 Ground State Problem*: Find the lowest eigenvalue and corresponding eigenvector(s) of* $\hat{H}$*.*

Proposition 1 *The operator* $\hat{N}_{\uparrow} \equiv \sum_i \hat{n}_{i\uparrow}$ *commutes with* $\hat{H}$*. So does the corresponding* $\hat{N}_{\downarrow}$ *operator.*

Proof 1 *The proof is left as an exercise to the reader. Note that due to the commutation, the ground state has a definite number of up and down electrons.*

II. RESULTS

A. Free System

Definition 17 *The problem stated in Definition 16 is called the free problem if* $U = 0$*. Likewise, we will talk about a free* $\hat{H}$ *when* $U = 0$*.*

Proposition 2 *The free problem belongs to* P*.*

Before the proof we need to define creation and destruction matrices.

Definition 18 The creation operator $\hat{c}^\dagger_{\uparrow,i} : \mathcal{V} \to \mathcal{V}$, *is given by (i) if* $x_i \& 1 = 0$ *then* $\hat{c}^\dagger_{\uparrow,i} \bigotimes_r |x_r\rangle = s_i \bigotimes_r |y_r\rangle$, *where* $y_r = x_r$ *if* $r \neq i$, *and* $y_i = x_i \wedge 1$, $s_i = (-1)^{\mathcal{N}_i \bigotimes_r |x_r\rangle}$ *and (ii)* $\emptyset$ *otherwise. Note that* $\mathcal{N}_i \bigotimes_r |x_r\rangle$ *is a natural number according to Definition 3. The destruction operator is the transpose conjugate of* $\hat{c}^\dagger$. *Similar definitions apply for* $\downarrow$.

Proof 2 *We will show how to construct the ground state, and will prove that the construction is polynomial in* N *and* N_e. *We assume that there are* $N_\uparrow$ *electrons with spin up, and* $N_\downarrow$ *electrons with spin down. The ground state of* $\hat{H}$ *when* $U = 0$ *is:*

$$\psi_{gs} = \prod_{m=0}^{m<N_\uparrow} \tilde{c}^\dagger_{m,\uparrow} \prod_{m=0}^{m<N_\downarrow} \tilde{c}^\dagger_{m\downarrow} |0, 0, ..., 0\rangle, \tag{5}$$

is the ground state of $\hat{H}$, *where*

$$\tilde{c}_{m,\sigma} = \sum_i W_{m,i} c_{i,\sigma}, \tag{6}$$

where W *are the eigenvectors of the* $N \times N$ *(hopping) matrix* t. *The ground state is* $E = E_\uparrow + E_\downarrow$, *where* $E_\uparrow = \sum_{m=0}^{m<N_\uparrow} \epsilon_m$, *and similarly for* $E_\downarrow$.

First, we will show that this construction is polynomial in N. *The computation of eigenvectors and eigenvalues of* t *is polynomial in* N, *since the rank of* t *is* N. *Construction eq. (6) has* N *terms and so is polynomial in* N. *Finally, construction eq. (5) is also polynomial in* N, *since it consists of the creation of electrons in a transformed-by-*W *space which is of size* N.

Finally, we show that Eq. (5) is indeed the ground state of $\hat{H}$. *From now on, and for simplicity, we forget about the down sector. This is possible since the two spin sectors decouple. FIXME COMPLETE THIS PART OF THE PROOF.*