Exact solution of the UCCD and UCCDQ angles for the 4-site Hubbard model at half-filling in momentum space

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1 The Hubbard Hamiltonian

The Hamiltonian of the Hubbard model in real space is given by:

$$H = -t \sum_{<ij>\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{1}$$

To get to the momentum space, we perform a Fourier transformation:

$$c^\dagger_{k\sigma} = \frac{1}{\sqrt{N}} \sum_j e^{ik\cdot r_j} c^\dagger_{j\sigma}, \tag{2}$$

$$c_{k\sigma} = \frac{1}{\sqrt{N}} \sum_j e^{-ik\cdot r_j} c_{j\sigma}, \tag{3}$$

where N is the number of sites. We then obtain the Hamiltonian in momentum space:

$$H = \sum_{k\sigma} \epsilon(k) c^\dagger_{k\sigma} c_{k\sigma} + \frac{U}{N} \sum_{k_1,k_2,k_3} c^\dagger_{k_1+k_2-k_3\uparrow} c_{k_2\uparrow} c^\dagger_{k_3\downarrow} c_{k_1\downarrow}, \tag{4}$$

where $\epsilon(k) = -2tcos(k)$. To obtain the ground state energy, we can use the exact diagonalization method. In the case we are currently working on, a four-site system at half-filling with $S_z = 0$, the ground state energy can be calculated exactly by solving the following equation:

$$E^3 - 3E^2U + 2E(U^2 - 8) + 24U = 0. \tag{5}$$

1.1 Numbering scheme and normal order

The four-site system we are working with has 2 up spins and 2 down spins, making the total number of basis elements $\binom{4}{2}\binom{4}{2} = 36$. For consistency and uniqueness, we need to define a normal order of numbering the elements and how we apply the operators to the states. First we use a string of eight binaries to represent the four momenta, the first four being the down spins, the second being the up spins. For example $|1,0,0,1\rangle\,|0,1,0,1\rangle$ represents a state where the a down spin has momentum $\frac{3\pi}{2}$, an up spin has momentum π, and a pair have momentum 0. We then assign an integer to each binary in the string, 1 to 8, from right to left. The order in which we apply the creation and annihilation operators in this work throughout is from higher to lower indices, i.e.,

$$c^\dagger_6 c^\dagger_7 c_5 c_8 \,|22\rangle$$

is not allowed. It needs to be

$$c^\dagger_7 c^\dagger_6 c_8 c_5 \,|22\rangle\,.$$

To number the 36 basis elements, we first number our string patterns:

$$0011 \rightarrow 1$$
$$0101 \rightarrow 2$$
$$0110 \rightarrow 3$$
$$1001 \rightarrow 4$$
$$1010 \rightarrow 5$$
$$1100 \rightarrow 6$$

we can then label each element by its indices (i, j), and combine them into $n = 6 \cdot (i-1) + j$. The example above, $|1,0,0,1\rangle\,|0,1,0,1\rangle$ should then be labeled $(4,2)$, which is equivalent to $6 \cdot (4-1) + 2 = 20$.

2 UCCD exact parameterization

(By working out all possible single excitations of both $|1\rangle$ and $|22\rangle$, and comparing them with the coefficients of the exact wavevector, we conclude that the UCCS angles are all zero.)
Jim has proven the identity:

$$e^{\theta(c_a^\dagger c_b^\dagger c_i c_j - c_i^\dagger c_j^\dagger c_b c_a)} = 1 + (cos(\theta) - 1)(n_a n_b n_i n_j - n_a n_b(n_i + n_j) - (n_a + n_b) n_i n_j + n_a n_b + n_i n_j) + sin(\theta)(c_a^\dagger c_b^\dagger c_i c_j - c_i^\dagger c_j^\dagger c_b c_a), \tag{6}$$

where a and b are indices of unoccupied momenta, and i and j are indices of occupied ones. Using this identity, we can show that

$$U_{i,j}^{a,b} |\psi_0\rangle = e^{\theta(c_a^\dagger c_b^\dagger c_i c_j - c_i^\dagger c_j^\dagger c_b c_a)} |\psi_0\rangle = cos(\theta) |\psi_0\rangle + sin(\theta) \left|\psi_{i,j}^{a,b}\right\rangle. \tag{7}$$

Due to the degeneracy of the ground state vector when $U = 0$, we instead use the ground state vector as $U \rightarrow 0$, and with our numbering scheme, the reference state to which we apply the UCC operators is:

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |22\rangle), \tag{8}$$

where $|1\rangle$ corresponds to the state $|00110011\rangle$, and $|22\rangle$ corresponds to $|10011001\rangle$. Therefore, we need two sets of UCC operators, one for $|1\rangle$, the other for $|22\rangle$. Below is a table for all possible states achieved by double excitations with respect to the two states. There are in total 36 $U_{i,j}^{a,b}$ operators we need to apply to the reference state $|\psi_0\rangle$, 18 for each. Using equation 7, we can show that

$$\left(\prod_{a,b,i,j} U_{i,j}^{a,b}\right) |\psi_0\rangle = \left(\prod_k cos(\theta_k)\right) |\psi_0\rangle + \sum_l \left(sin(\theta_l)(\prod_{k \neq l} cos(\theta_k)) |\psi_l\rangle\right), \tag{9}$$

where k and l are short-handed for distinct sets of a, b, i, j, and $|\psi_l\rangle$ represents the state after which we apply the double excitation operator $c_a^\dagger c_b^\dagger c_i c_j - c_i^\dagger c_j^\dagger c_b c_a$, with a, b, i, j corresponds to the short-hand notation l. Further, we can show that equation 9 becomes

$$\left(\prod_{k=1}^{18} cos(\theta_k)\right) |1\rangle + \sum_{l=1}^{18} \left(sin(\theta_l)(\prod_{k \neq l} cos(\theta_k)) |1\rangle\right) - \left(\prod_{k=19}^{36} cos(\theta_k)\right) |22\rangle - \sum_{l=19}^{36} \left(sin(\theta_l)(\prod_{k \neq l} cos(\theta_k)) |22\rangle\right) \tag{10}$$

l	$\lvert i \to j; k \to l\rangle$	$\lvert\psi_l\rangle$	$\lvert i \uparrow j \uparrow k \downarrow l \downarrow\rangle$
1	$\lvert 0 \to 2; 0 \to 2\rangle$	$-\lvert 15\rangle$	$-\lvert 2 \uparrow 1 \uparrow 2 \downarrow 1 \downarrow\rangle$
6	$\lvert 1 \to 3; 0 \to 2\rangle$	$\lvert 16\rangle$	$\lvert 3 \uparrow 0 \uparrow 2 \downarrow 1 \downarrow\rangle$
7	$\lvert 1 \to 2; 0 \to 3\rangle$	$\lvert 26\rangle$	$\lvert 2 \uparrow 0 \uparrow 3 \downarrow 1 \downarrow\rangle$
10	$\lvert 0 \to 3; 1 \to 2\rangle$	$\lvert 11\rangle$	$\lvert 3 \uparrow 1 \uparrow 2 \downarrow 0 \downarrow\rangle$
11	$\lvert 0 \to 2; 1 \to 3\rangle$	$\lvert 21\rangle$	$\lvert 2 \uparrow 1 \uparrow 3 \downarrow 0 \downarrow\rangle$
17	$\lvert 0 \to 2, 1 \to 3;\rangle$	$-\lvert 6\rangle$	$-\lvert 3 \uparrow 2 \uparrow 1 \downarrow 0 \downarrow\rangle$
18	$\lvert ; 0 \to 2, 1 \to 3\rangle$	$-\lvert 31\rangle$	$-\lvert 1 \uparrow 0 \uparrow 3 \downarrow 2 \downarrow\rangle$
22	$\lvert 0 \to 2; 0 \to 2\rangle$	$-\lvert 36\rangle$	$-\lvert 3 \uparrow 2 \uparrow 3 \downarrow 2 \downarrow\rangle$
24	$\lvert 3 \to 2; 0 \to 1\rangle$	$-\lvert 26\rangle$	$-\lvert 2 \uparrow 0 \uparrow 3 \downarrow 1 \downarrow\rangle$
25	$\lvert 3 \to 1; 0 \to 2\rangle$	$-\lvert 31\rangle$	$-\lvert 1 \uparrow 0 \uparrow 3 \downarrow 2 \downarrow\rangle$
28	$\lvert 0 \to 2; 3 \to 1\rangle$	$-\lvert 6\rangle$	$-\lvert 3 \uparrow 2 \uparrow 1 \downarrow 0 \downarrow\rangle$
29	$\lvert 0 \to 1; 3 \to 2\rangle$	$-\lvert 11\rangle$	$-\lvert 3 \uparrow 1 \uparrow 2 \downarrow 0 \downarrow\rangle$
35	$\lvert 0 \to 1, 3 \to 2;\rangle$	$-\lvert 21\rangle$	$-\lvert 2 \uparrow 1 \uparrow 3 \downarrow 0 \downarrow\rangle$
36	$\lvert ; 0 \to 1, 3 \to 2\rangle$	$-\lvert 16\rangle$	$-\lvert 3 \uparrow 0 \uparrow 2 \downarrow 1 \downarrow\rangle$

After expanding equation 10, and comparing the coefficients with the exact ground state vector, we manage to get a system of equations:

$$x_1x_6x_7x_{10}x_{11}x_{17}x_{18} = c_1(\alpha_{1\uparrow0\uparrow1\downarrow0\downarrow}), \tag{11}$$

$$-x_1x_6x_7x_{10}x_{11}x_{18}\sqrt{1-x_{17}^2} + x_{22}x_{24}x_{25}x_{29}x_{35}x_{36}\sqrt{1-x_{28}^2} = c_6(\alpha_{3\uparrow2\uparrow1\downarrow0\downarrow}), \tag{12}$$

$$x_1x_6x_7x_{11}x_{17}x_{18}\sqrt{1-x_{10}^2} + x_{22}x_{24}x_{25}x_{28}x_{35}x_{36}\sqrt{1-x_{29}^2} = c_{11}(\alpha_{3\uparrow1\uparrow2\downarrow0\downarrow}), \tag{13}$$

$$-x_6x_7x_{10}x_{11}x_{17}x_{18}\sqrt{1-x_1^2} = c_{15}(-\alpha_{2\uparrow1\uparrow2\downarrow1\downarrow}), \tag{14}$$

$$x_1x_7x_{10}x_{11}x_{17}x_{18}\sqrt{1-x_6^2} + x_{22}x_{24}x_{25}x_{28}x_{29}x_{35}\sqrt{1-x_{36}^2} = c_{16}(\alpha_{3\uparrow0\uparrow2\downarrow1\downarrow}), \tag{15}$$

$$x_1x_6x_7x_{10}x_{17}x_{18}\sqrt{1-x_{11}^2} + x_{22}x_{24}x_{25}x_{28}x_{29}x_{36}\sqrt{1-x_{35}^2} = c_{21}(\alpha_{2\uparrow1\uparrow3\downarrow0\downarrow}), \tag{16}$$

$$-x_{22}x_{24}x_{25}x_{28}x_{29}x_{35}x_{36} = c_{22}(-\alpha_{3\uparrow0\uparrow3\downarrow0\downarrow}), \tag{17}$$

$$x_1x_6x_{10}x_{11}x_{17}x_{18}\sqrt{1-x_7^2} + x_{22}x_{25}x_{28}x_{29}x_{35}x_{36}\sqrt{1-x_{24}^2} = c_{26}(\alpha_{2\uparrow0\uparrow3\downarrow1\downarrow}), \tag{18}$$

$$-x_1x_6x_7x_{10}x_{11}x_{17}\sqrt{1-x_{18}^2} + x_{22}x_{24}x_{28}x_{29}x_{35}x_{36}\sqrt{1-x_{25}^2} = c_{31}(\alpha_{1\uparrow0\uparrow3\downarrow2\downarrow}), \tag{19}$$

$$x_{24}x_{25}x_{28}x_{29}x_{35}x_{36}\sqrt{1-x_{22}^2} = c_{36}(\alpha_{3\uparrow2\uparrow3\downarrow2\downarrow}), \tag{20}$$

where $x_i = cos\theta_i$, and with the boundary conditions:

$$c_1 = -c_{22} = \alpha, \tag{21}$$

$$c_6 = c_{16} = c_{21} = c_{31} = \beta \tag{22}$$

$$c_{11} = c_{26} = 2c_6 = 2\alpha, \tag{23}$$

$$c_{15} = -c_{36} = \gamma. \tag{24}$$

Based on equation 21, equation 11, and equation 17, it is obvious that

$$x_1x_6x_7x_{10}x_{11}x_{17}x_{18} = x_{22}x_{24}x_{25}x_{28}x_{29}x_{35}x_{36} = \alpha. \tag{25}$$

We will then make some educated guesses:

$$x_{10} = x_7, \tag{26}$$
$$x_{29} = x_{24}, \tag{27}$$
$$x_{17} = x_{18}, \tag{28}$$
$$x_{28} = x_{25}, \tag{29}$$
$$x_1 = x_{22}, \tag{30}$$
$$x_6 = x_{11}, \tag{31}$$
$$xx_{36} = x_{35}. \tag{32}$$

based on equation 11, 13, 14, 15, 16, 17, and 18, and boundary conditions 21, 22, 23, and 24. Further, we look at equation 22 and 23, and conclude that:

$$x_{10} = 2x_6. \tag{33}$$

Because of the minus sign infront of equation 12 and 19, it is obvious that

$$x_{17} = x_{18} = -x_6. \tag{34}$$

Therefore, we sort everything out and have the following relations between variables:

$$x_7 = x_{10} = x_{24} = x_{29} = 2x_6, \tag{35}$$
$$x_6 = x_{11} = x_{25} = x_{28} = x_{35} = x_{36}, \tag{36}$$
$$x_1 = x_{22}, \tag{37}$$
$$x_{17} = x_{18} = -x_6. \tag{38}$$

One can easily substitute those into the original system of equations and verify they satisfy the boundary conditions.

Thus, the high symmetricity of the exact wavevectors help us reduce the system to a minimum of 3 equations:

$$4x_1x_6^6 = \alpha, \tag{39}$$
$$8x_1x_6^5\sqrt{1-x_6^2} = \beta, \tag{40}$$
$$-4\sqrt{1-x_1^2}x_6^6 = \gamma. \tag{41}$$

Thus, the four distinct values of the angles are:

$$\theta_{22} = \theta_1 = arctan(\frac{-\gamma}{\alpha}), \tag{42}$$
$$\theta_{11} = \theta_{25} = \theta_{28} = \theta_{35} = \theta_{36} = \theta_6 = arctan(\frac{\beta}{2\alpha}), \tag{43}$$
$$\theta_{10} = \theta_{24} = \theta_{29} = \theta_7 = 2\theta_6, \tag{44}$$
$$\theta_{17} = \theta_{18} = -\theta_6, \tag{45}$$

and all other θ are exactly zero.

3 UCCDQ exact parameterization

By carefully working out all possible triple excitations of all $|\psi_l\rangle$ with nonzero coefficients after applying the UCCD operators, and comparing them with the coefficients of the exact wavevector, we conclude

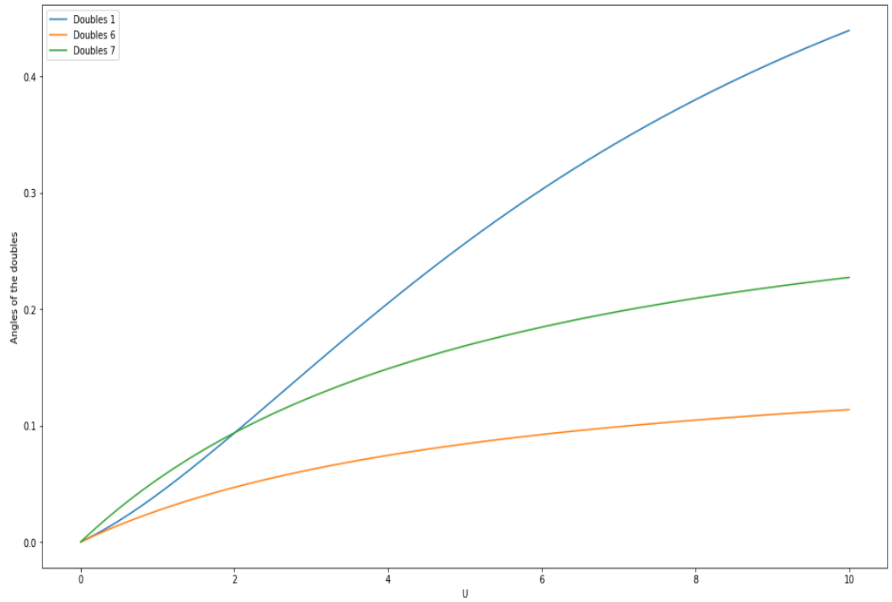

Figure 1: The three distinct angles vs. U

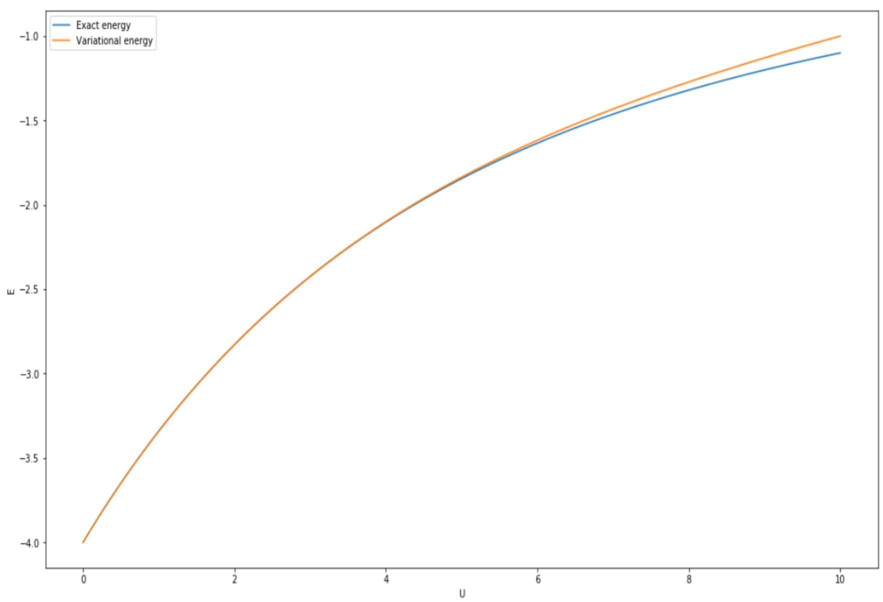

Figure 2: The variational energy of the wavevectors obtained by applying the UCCD operator in the factorized form vs. U

that the triples angles are all zero.
Similar to equation 7, we can derive that

$$U_{i,j,k,l}^{a,b,c,d} |\psi_0\rangle = e^{\theta(c_a^\dagger c_b^\dagger c_c^\dagger c_d^\dagger c_i c_j c_k c_l - c_i^\dagger c_j^\dagger c_k^\dagger c_l^\dagger c_d c_c c_b c_a)} |\psi_0\rangle = cos(\theta) |\psi_0\rangle + sin(\theta) \left|\psi_{i,j,k,l}^{a,b,c,d}\right\rangle. \tag{46}$$

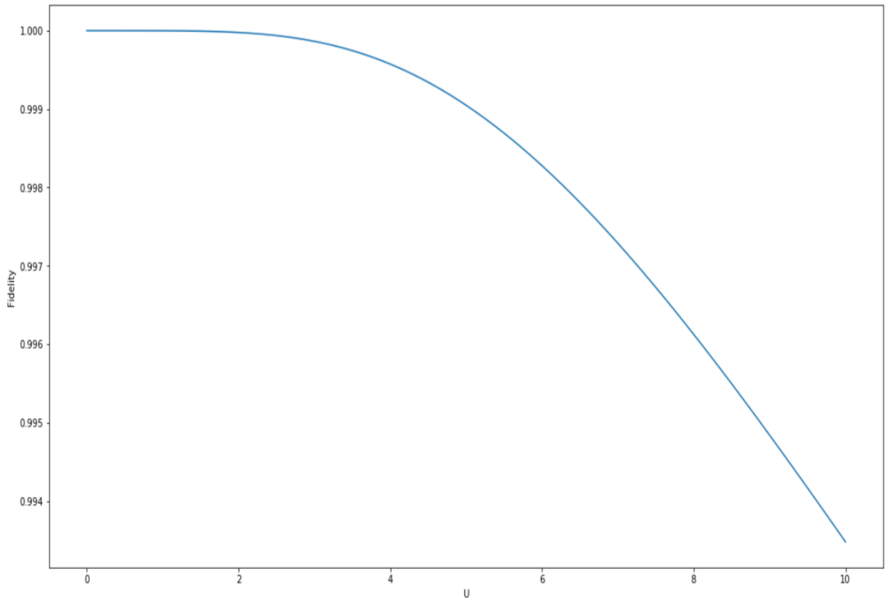

Figure 3: Fidelity of the UCCD anzats with the exact solution vs. U

$\|1\rangle \rightarrow \|36\rangle$	$\|21\rangle \rightarrow \|16\rangle$
$\|6\rangle \rightarrow \|31\rangle$	$\|22\rangle \rightarrow \|15\rangle$
$\|11\rangle \rightarrow \|26\rangle$	$\|26\rangle \rightarrow \|11\rangle$
$\|15\rangle \rightarrow \|22\rangle$	$\|31\rangle \rightarrow \|6\rangle$
$\|16\rangle \rightarrow \|21\rangle$	$\|36\rangle \rightarrow \|1\rangle$

Above is a table for the quadruple excitations. After expanding the UCCDQ in product form into *cos* and *sin* terms, we reach a system of transcendental equations:

$$c_{1D} cos\theta_1 - c_{15D} sin\theta_{15} = c_1, \tag{47}$$

$$c_{6D}(cos\theta_6 + sin\theta_6) = c_6, \tag{48}$$

$$c_{15D} cos\theta_{15} - c_{1D} sin\theta_1 = c_{15}, \tag{49}$$

$$cos\theta_{11} + sin\theta_{11} = 2(cos\theta_6 + sin\theta_6), \tag{50}$$

where c_{iD} represents the coefficient of i-th term in the UCCD wavevector. Equation 34 and 36 can be solved sequentially, but the other two must be solved simultaneously, producing 8 distinct sets of solutions. I have yet to establish a systematic way of determining which set to use for different U values. One can try to write down the exact solutions for θ_1 and θ_{15}, but they are highly nontrivial, each with at least 256 terms. The way that probably works is to find the roots numerically. One good news is that if we solved equation 34 and 36, the coefficients will match those in the exact wavefunction (before doing any normalization). And since the other coefficients are all zero, we can say with great confidence that if we solved all four equations, we will get an exact wavevector just by applying UCCDQ operators to $|\psi_0\rangle$.