

.....

.....

(.....)

.....

# 1 Exact diagonalization of the two-site Hubbard model

## The Hamiltonian

$$\mathcal{H} = -t \sum_{\sigma} \left( c_{1\sigma}^{\dagger} c_{2\sigma} + c_{2\sigma}^{\dagger} c_{1\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \hat{N} \quad (1)$$

I have two lattice sites, indexed by 1 and 2, occupied by electrons.  $\mu$  is the chemical potential,  $c_{i\sigma}^{\dagger}$  and  $c_{i\sigma}$  are the fermionic creation and annihilation operators at the  $i^{\text{th}}$  site, with spin-index  $\sigma$ .  $\sigma$  can take values  $\uparrow$  and  $\downarrow$ , denoting spin-up and spin-down states respectively.  $\hat{n}_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$  is the number operator for the  $i^{\text{th}}$  site and at spin-index  $\sigma$ ; it counts the number of fermions with the designated quantum numbers.  $\hat{N} = \sum_{i\sigma} \hat{n}_{i\sigma}$  is the total number operator; it counts the total number of fermions at all sites and spin-indices.  $t$  is the hopping strength; the more the  $t$ , the more are the electrons likely to hop between sites.  $U$  is the on-site repulsion cost; it represents the increase in energy when two electrons occupy the same site.

## 1.1 Symmetries of the problem

The following operators commute with the Hamiltonian.

1. **Total number operator**  $\hat{N}$ :  $[\mathcal{H}, \hat{N}] = 0$ . The proof is as follows: The last term in the Hamiltonian is the number operator itself. Ignoring that, there are three terms that I need to individually consider.

- $c_{1\sigma}^{\dagger} c_{2\sigma}$

$$\begin{aligned} [c_{1\sigma}^{\dagger} c_{2\sigma}, \hat{n}_{i\sigma'}] &= [c_{1\sigma}^{\dagger} c_{2\sigma}, c_{i\sigma'}^{\dagger} c_{i\sigma'}] \\ &= c_{1\sigma}^{\dagger} [c_{2\sigma}, c_{i\sigma'}^{\dagger} c_{i\sigma'}] + [c_{1\sigma}^{\dagger}, c_{i\sigma'}^{\dagger} c_{i\sigma'}] c_{2\sigma} \\ &= \delta_{i,2} c_{1\sigma}^{\dagger} [c_{2\sigma}, c_{2\sigma'}^{\dagger} c_{2\sigma'}] + \delta_{i,1} [c_{1\sigma}^{\dagger}, c_{1\sigma'}^{\dagger} c_{1\sigma'}] c_{2\sigma} \\ &= \delta_{i,2} c_{1\sigma}^{\dagger} \{c_{2\sigma}, c_{2\sigma'}^{\dagger}\} c_{2\sigma'} - \delta_{i,1} c_{1\sigma}^{\dagger} \{c_{1\sigma'}, c_{1\sigma}^{\dagger}\} c_{2\sigma} \\ &= \delta_{\sigma,\sigma'} c_{1\sigma}^{\dagger} c_{1\sigma} (\delta_{i,2} - \delta_{i,1}) \end{aligned} \quad (2)$$

The third line follows because the electrons on different sites are distinguishable and hence, the *creation and annihilation operators of different sites will commute among themselves*. Therefore,

$$[c_{1\sigma}^{\dagger} c_{2\sigma}, \hat{N}] = \sum_{i\sigma'} [c_{1\sigma}^{\dagger} c_{2\sigma}, \hat{n}_{i\sigma'}] = c_{1\sigma}^{\dagger} c_{1\sigma} \sum_{i=\{1,2\}} (\delta_{i,2} - \delta_{i,1}) = 0 \quad (3)$$

- $c_{2\sigma}^{\dagger} c_{1\sigma}$ : Since the operator  $\hat{N}$  is symmetric with respect to the site indices 1 and 2, I can go through the last proof again with the site indices 1 and 2 exchanged and since the proof does not depend on the site indices, this commutator will also be zero.

- $\hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$ :

$$\begin{aligned} [\hat{n}_{i\uparrow} \hat{n}_{j\downarrow}, \hat{n}_{j\sigma}] &= \hat{n}_{i\uparrow} [\hat{n}_{j\downarrow}, \hat{n}_{j\sigma}] - [\hat{n}_{i\uparrow}, \hat{n}_{j\sigma}] \hat{n}_{j\downarrow} \\ &= \delta_{ij} (\hat{n}_{i\uparrow} [\hat{n}_{i\downarrow}, \hat{n}_{i\sigma}] - [\hat{n}_{i\uparrow}, \hat{n}_{i\sigma}] \hat{n}_{i\downarrow}) \\ &= \delta_{ij} (\delta_{\sigma\uparrow} \hat{n}_{i\uparrow} [\hat{n}_{i\downarrow}, \hat{n}_{i\uparrow}] - \delta_{\sigma\downarrow} [\hat{n}_{i\uparrow}, \hat{n}_{i\downarrow}] \hat{n}_{i\downarrow}) \\ &= \delta_{ij} (\delta_{\sigma\downarrow} \hat{n}_{i\downarrow} - \delta_{\sigma\uparrow} \hat{n}_{i\uparrow}) [\hat{n}_{i\uparrow}, \hat{n}_{i\downarrow}] \\ &= \delta_{ij} (\delta_{\sigma\downarrow} \hat{n}_{i\downarrow} - \delta_{\sigma\uparrow} \hat{n}_{i\uparrow}) (c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow} - c_{i\downarrow}^{\dagger} c_{i\downarrow} c_{i\uparrow}^{\dagger} c_{i\uparrow}) \\ &= \delta_{ij} (\delta_{\sigma\downarrow} \hat{n}_{i\downarrow} - \delta_{\sigma\uparrow} \hat{n}_{i\uparrow}) (c_{i\downarrow}^{\dagger} c_{i\downarrow} c_{i\uparrow}^{\dagger} c_{i\uparrow} - c_{i\downarrow}^{\dagger} c_{i\downarrow} c_{i\uparrow}^{\dagger} c_{i\uparrow}) = 0 \end{aligned} \quad (4)$$

Therefore,  $[\hat{n}_{i\uparrow} \hat{n}_{j\downarrow}, \hat{N}] = \sum_{j,\sigma} [\hat{n}_{i\uparrow} \hat{n}_{j\downarrow}, \hat{n}_{j\sigma}] = 0$

The total Hamiltonian is just a sum of the three terms; since the number operator commutes individually with these terms, it obviously commutes with the total Hamiltonian. QED

2. **Magnetization operator**  $\hat{S}_{tot}^z$ :  $\hat{S}_{tot}^z \equiv \frac{1}{2} \sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$ ,  $[\mathcal{H}, \hat{S}_{tot}^z] = 0$ . This proof goes as follows.

The magnetization operator can be rewritten as  $\hat{S}_{tot}^z = \frac{1}{2} \sum_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} - 2\hat{n}_{i\downarrow}) = \hat{N} - 2 \sum_i \hat{n}_{i\downarrow}$ . Since  $\hat{N}$  commutes with  $\mathcal{H}$ , I just need to prove that  $[\mathcal{H}, \sum_i \hat{n}_{i\downarrow}] = 0$ . From eq. 2,

$$\left[ c_{1\sigma}^\dagger c_{2\sigma}, \sum_i \hat{n}_{i\downarrow} \right] = c_{1\downarrow}^\dagger c_{1\downarrow} \sum_{i=\{1,2\}} (\delta_{i,2} - \delta_{i,1}) = 0 \quad (5)$$

Again using the symmetry of the magnetization operator with the exchange of indices, its obvious that  $\left[ c_{2\sigma}^\dagger c_{1\sigma}, \sum_i \hat{n}_{i\downarrow} \right] = 0$

Using eq. 4,  $[\hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \hat{n}_{i\downarrow}] = 0$ .

Finally,  $[N, \hat{n}_{i\downarrow}] = \sum_{j\sigma} [\hat{n}_{j\sigma}, \hat{n}_{i\downarrow}] = [\hat{n}_{i\uparrow}, \hat{n}_{i\downarrow}] = c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} - c_{i\downarrow}^\dagger c_{i\downarrow} c_{i\uparrow}^\dagger c_{i\uparrow} = 0$ . Since  $\hat{S}_{tot}^z$  commutes with each part individually, it commutes with the total Hamiltonian. QED

3. **Two-site parity operator**  $\hat{P}$ : The action of  $\hat{P}$  is defined as follows. If  $|\psi_{\alpha\beta}\rangle$  is a wavefunction with site indices  $\alpha$  and  $\beta$ ,

$$\hat{P} |\psi(\alpha, \beta)\rangle = |\psi(\beta, \alpha)\rangle \quad (6)$$

That is, it operates on each electron and reverses it's site indices. I now rewrite the Hamiltonian by explicitly showing the two site indices:

$$\mathcal{H}(\alpha, \beta) = -t \sum_{\sigma} (c_{\alpha\sigma}^\dagger c_{\beta\sigma} + c_{\beta\sigma}^\dagger c_{\alpha\sigma}) + U(n_{\alpha\uparrow} n_{\alpha\downarrow} + n_{\beta\uparrow} n_{\beta\downarrow}) - \mu \sum_{\sigma} (n_{\alpha\sigma} + n_{\beta\sigma}) \quad (7)$$

Its obvious that  $\mathcal{H}$  is symmetric in the site indices:  $\mathcal{H}(\alpha, \beta) = \mathcal{H}(\beta, \alpha)$ . This means that the eigenvalues also have this symmetry. Let  $|\phi(\alpha, \beta)\rangle$  be an eigenstate of  $\mathcal{H}(\alpha, \beta)$  with eigenvalue  $E(\alpha, \beta)$ . Then,

$$\hat{P} \mathcal{H} |\phi(\alpha, \beta)\rangle = E(\alpha, \beta) \hat{P} |\phi(\alpha, \beta)\rangle = E(\beta, \alpha) |\psi(\beta, \alpha)\rangle = \mathcal{H} |\psi(\beta, \alpha)\rangle = \mathcal{H} \hat{P} |\psi(\alpha, \beta)\rangle \quad (8)$$

$$\mathcal{H}(\alpha, \beta) \hat{P} |\phi(\alpha, \beta)\rangle = \mathcal{H}(\alpha, \beta) |\phi(\beta, \alpha)\rangle \quad (9)$$

Since any general wavefunction can be expanded in terms of these wavefunctions and since both the operator are linear, the above result will also hold for a general wavefunction  $|\psi(\alpha, \beta)\rangle$ :

$$\mathcal{H} \hat{P} |\psi(\alpha, \beta)\rangle = \hat{P} \mathcal{H} |\psi(\alpha, \beta)\rangle \implies [\mathcal{H}, \hat{P}] = 0 \quad (10)$$

## 1.2 Partitioning the Hilbert space

The Hamiltonian commutes with the three operators. This means that is possible to simultaneously diagonalize these four operators:  $\mathcal{H}, \hat{N}, \hat{S}_z^{tot}, \hat{P}$ . I will be able to label the eigenstates of the total Hamiltonian using the eigenvalues of these operators. First take the total number operator.  $\hat{N}$  can take four values for a two-site system, 1 through 4. The eigenstates labelled by a particular number, say  $N=2$  will be orthogonal to the eigenstates labelled by another number, say  $N=4$ . This means each eigenvalue of  $\hat{N}$  will have a distinct subspace orthogonal to the other values of  $\hat{N}$ . I will be able to diagonalize each such subspace independently of each other, because they will not have any overlap. This feature enables us to block-diagonalize the total Hamiltonian into four blocks, each block belonging to each value  $\hat{N}$ .

Inside each block, I will be able to repeat the procedure by next using the eigenvalues of  $\hat{S}_z^{tot}$ . Each block of the Hamiltonian will again break up to smaller blocks for each value of the total magnetization. The eigenvalues of parity operator provide a further partitioning of the blocks of magnetization.

From this point, all the states I will work with will necessarily be eigenfunctions of  $\hat{N}$ , so it doesn't make sense to keep the last term in the Hamiltonian,  $\mu \hat{N}$ . I redefine the Hamiltonian by absorbing this term:  $\mathcal{H} \rightarrow \mathcal{H} + \mu \hat{N} = -t \sum_{\sigma} (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$ . This will keep the eigenvectors unaltered, but will increase the eigenvalues by  $\mu N$ , where  $N$  is the number of particles in the eigenstate I are considering.

### 1.3 N = 1

For writing the state kets, I use the following notation:  $|\uparrow, \downarrow\rangle$  means electron on site 1 has spin up and that on site 2 has spin-down.  $|\downarrow, 0\rangle$  means electron on site 1 has spin-down and there is no electron on site 2.

For one electron on two lattice sites, I start by writing down the eigenstates of  $S_z^{tot}$ . For odd number of electrons, zero magnetization is not possible. So,

- $S_z^{tot} = -1$ :  $|\downarrow, 0\rangle, |0, \downarrow\rangle$
- $S_z^{tot} = +1$ :  $|\uparrow, 0\rangle, |0, \uparrow\rangle$

Each eigenvalue will have a separate subspace and can be separately diagonalized. I need to find the matrix elements of  $\mathcal{H}$  in these eigenkets. Since there is no possibility of two electrons occupying same site, I ignore the  $U$ -term for the time being.

#### 1.3.1 $S_z^{tot} = -1$

Let us first see the action of the Hamiltonian on the eigenfunctions with  $S_z^{tot} = -1$ .

$$\begin{aligned}\mathcal{H}|\downarrow, 0\rangle &= -tc_{2\downarrow}^\dagger c_{1\downarrow}|\downarrow, 0\rangle = -t|0, \downarrow\rangle \\ \mathcal{H}|0, \downarrow\rangle &= -tc_{1\downarrow}^\dagger c_{2\downarrow}|0, \downarrow\rangle = -t|\downarrow, 0\rangle\end{aligned}\tag{11}$$

We get the following matrix for this tiny subspace of the Hamiltonian:

$$\begin{array}{c} \begin{array}{cc} |\downarrow, 0\rangle & |0, \downarrow\rangle \\ \begin{array}{c} |\downarrow, 0\rangle \\ |0, \downarrow\rangle \end{array} \left( \begin{array}{cc} 0 & -t \\ -t & 0 \end{array} \right) \end{array}\tag{12}$$

The eigenvalues and eigenvectors of this matrix are  $\frac{|\downarrow, 0\rangle \pm |0, \downarrow\rangle}{\sqrt{2}}$ , with eigenvalues  $\mp t$ . These are also the eigenvalues of the parity operator, as expected.

$$\begin{aligned}\hat{P}(|\downarrow, 0\rangle + |0, \downarrow\rangle) &= |0, \downarrow\rangle + |\downarrow, 0\rangle \implies \hat{P} = 1 \\ \hat{P}(|\downarrow, 0\rangle - |0, \downarrow\rangle) &= |0, \downarrow\rangle - |\downarrow, 0\rangle \implies \hat{P} = -1\end{aligned}\tag{13}$$

#### 1.3.2 $S_z^{tot} = +1$

Now I look at the spin-up states.

$$\begin{aligned}\mathcal{H}|\uparrow, 0\rangle &= -tc_{2\uparrow}^\dagger c_{1\uparrow}|\uparrow, 0\rangle = -t|0, \uparrow\rangle \\ \mathcal{H}|0, \uparrow\rangle &= -tc_{1\uparrow}^\dagger c_{2\uparrow}|0, \uparrow\rangle = -t|\uparrow, 0\rangle\end{aligned}\tag{14}$$

Clearly, this gives the same matrix as the spin-down states:

$$\begin{array}{c} \begin{array}{cc} |\uparrow, 0\rangle & |0, \uparrow\rangle \\ \begin{array}{c} |\uparrow, 0\rangle \\ |0, \uparrow\rangle \end{array} \left( \begin{array}{cc} 0 & -t \\ -t & 0 \end{array} \right) \end{array}\tag{15}$$

and hence similar eigenfunctions:  $\frac{|\uparrow, 0\rangle \pm |0, \uparrow\rangle}{\sqrt{2}}$ , with eigenvalues  $\mp t$ .

## 1.4 N=3

I once again write down the eigenstates of  $S_z^{tot}$ , this time with three electrons.

- $S_z^{tot} = -1$ :  $|\uparrow\downarrow, \downarrow\rangle, |\downarrow, \uparrow\downarrow\rangle$
- $S_z^{tot} = +1$ :  $|\uparrow\downarrow, \uparrow\rangle, |\uparrow, \uparrow\downarrow\rangle$

**1.4.1**  $S_z^{tot} = -1$

$$\begin{aligned}\mathcal{H}|\uparrow\downarrow, \downarrow\rangle &= -tc_{2\uparrow}^\dagger c_{1\uparrow}|\uparrow\downarrow, \downarrow\rangle + U|\uparrow\downarrow, \downarrow\rangle = -t|\downarrow, \uparrow\downarrow\rangle + U|\uparrow\downarrow, \downarrow\rangle \\ \mathcal{H}|\downarrow, \uparrow\downarrow\rangle &= -tc_{1\uparrow}^\dagger c_{2\uparrow}|\downarrow, \uparrow\downarrow\rangle + U|\downarrow, \uparrow\downarrow\rangle = -t|\uparrow\downarrow, \downarrow\rangle + U|\downarrow, \uparrow\downarrow\rangle\end{aligned}\tag{16}$$

$$\begin{array}{c} |\uparrow\downarrow, \downarrow\rangle \quad |\downarrow, \uparrow\downarrow\rangle \\ |\uparrow\downarrow, \downarrow\rangle \begin{pmatrix} U & -t \\ -t & U \end{pmatrix} \\ |\downarrow, \uparrow\downarrow\rangle \end{array}\tag{17}$$

This matrix has eigenvalues  $U \mp t$ , and corresponding eigenvectors  $\frac{|\uparrow\downarrow, \downarrow\rangle \pm |\downarrow, \uparrow\downarrow\rangle}{\sqrt{2}}$

**1.4.2**  $S_z^{tot} = +1$

$$\begin{aligned}\mathcal{H}|\uparrow\downarrow, \uparrow\rangle &= -tc_{2\downarrow}^\dagger c_{1\downarrow}|\uparrow\downarrow, \uparrow\rangle + U|\uparrow\downarrow, \uparrow\rangle = tc_{2\downarrow}^\dagger c_{1\downarrow}|\downarrow\uparrow, \uparrow\rangle + U|\uparrow\downarrow, \uparrow\rangle \\ &= t|\uparrow, \downarrow\uparrow\rangle + U|\uparrow\downarrow, \uparrow\rangle = -t|\uparrow, \uparrow\downarrow\rangle + U|\uparrow\downarrow, \uparrow\rangle \\ \mathcal{H}|\uparrow, \uparrow\downarrow\rangle &= -tc_{1\downarrow}^\dagger c_{2\downarrow}|\uparrow, \uparrow\downarrow\rangle + U|\uparrow, \uparrow\downarrow\rangle = tc_{1\downarrow}^\dagger c_{2\downarrow}|\uparrow, \downarrow\uparrow\rangle + U|\uparrow, \uparrow\downarrow\rangle \\ &= t|\downarrow\uparrow, \uparrow\rangle + U|\uparrow, \uparrow\downarrow\rangle = -t|\uparrow\downarrow, \uparrow\rangle + U|\uparrow, \uparrow\downarrow\rangle\end{aligned}\tag{18}$$

$$\begin{array}{c} |\uparrow\downarrow, \uparrow\rangle \quad |\uparrow, \uparrow\downarrow\rangle \\ |\uparrow\downarrow, \uparrow\rangle \begin{pmatrix} U & -t \\ -t & U \end{pmatrix} \\ |\uparrow, \uparrow\downarrow\rangle \end{array}\tag{19}$$

This matrix has eigenvalues  $U \mp t$ , and corresponding eigenvectors  $\frac{|\uparrow\downarrow, \uparrow\rangle \pm |\uparrow, \uparrow\downarrow\rangle}{\sqrt{2}}$

## 1.5 N=4

With four electrons, the only possible state is  $|\uparrow\downarrow, \uparrow\downarrow\rangle$ . Its easy to find the eigenvalue. Since all states are filled, no hopping can take place, so the hopping term is zero. Therefore,

$$\mathcal{H}|\uparrow\downarrow, \uparrow\downarrow\rangle = 2U|\uparrow\downarrow, \uparrow\downarrow\rangle\tag{20}$$

So,  $|\uparrow\downarrow, \uparrow\downarrow\rangle$  is an eigenvector with eigenvalue  $2U$ .

## 1.6 N=2

This is the eigenvalue that has the largest subspace.

- $S_z^{tot} = -1$ :  $|\downarrow, \downarrow\rangle$
- $S_z^{tot} = +1$ :  $|\uparrow, \uparrow\rangle$
- $S_z^{tot} = 0$ :  $|\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle, |0, \uparrow\downarrow\rangle, |\uparrow\downarrow, 0\rangle$

### 1.6.1 $S_z^{tot} = \pm 1$

These two subspaces have a single state each, so they are obviously eigenstates. Since they both have identical spins on both sites, the hopping term is 0, and the  $U$ -term is also zero because of single occupation. As a result, they both have zero eigenvalue

$$\mathcal{H} |\downarrow, \downarrow\rangle = \mathcal{H} |\uparrow, \uparrow\rangle = 0 \quad (21)$$

### 1.6.2 $S_z^{tot} = 0$

This subspace has four eigenvectors,

$$|\uparrow, \downarrow\rangle, \quad |\downarrow, \uparrow\rangle, \quad |0, \uparrow\downarrow\rangle, \quad |\uparrow\downarrow, 0\rangle \quad (22)$$

so it is not possible to directly diagonalize this subspace. First we organize these states into eigenstates of parity. It is easy by inspection.

$$\begin{aligned} \hat{P} (|\uparrow, \downarrow\rangle \pm |\downarrow, \uparrow\rangle) &= \pm (|\uparrow, \downarrow\rangle \pm |\downarrow, \uparrow\rangle) \\ \hat{P} (|\uparrow\downarrow, 0\rangle \pm |0, \uparrow\downarrow\rangle) &= \pm (|\uparrow\downarrow, 0\rangle \pm |0, \uparrow\downarrow\rangle) \end{aligned} \quad (23)$$

I have the parity eigenstates for this subspace, so its most convenient to work in the basis of these eigenstates

- $\hat{P} = 1 : \frac{|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle}{\sqrt{2}}, \quad \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}}$
- $\hat{P} = -1 : \frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}}, \quad \frac{|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle}{\sqrt{2}}$

Each eigenvalue subspace can now be diagonalized separately. First I look at the eigenstates of  $\hat{P} = 1$ . I find the matrix of  $\mathcal{H}$  in the subspace spanned by these two vectors and then diagonalize that subspace.

$$\begin{aligned} \mathcal{H} \frac{|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}} \left\{ (c_{1\downarrow}^\dagger c_{2\downarrow} + c_{2\uparrow}^\dagger c_{1\uparrow}) |\uparrow, \downarrow\rangle + (c_{1\uparrow}^\dagger c_{2\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow}) |\downarrow, \uparrow\rangle \right\} \\ &= -\frac{t}{\sqrt{2}} \{ |\downarrow\uparrow, 0\rangle + |0, \uparrow\downarrow\rangle + |\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle \} = 0 \\ \mathcal{H} \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}} \left\{ (c_{2\uparrow}^\dagger c_{1\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow}) |\uparrow\downarrow, 0\rangle + (c_{1\uparrow}^\dagger c_{2\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow}) |0, \uparrow\downarrow\rangle \right\} + U \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \\ &= -\frac{t}{\sqrt{2}} \{ |\downarrow, \uparrow\rangle - |\uparrow, \downarrow\rangle + |\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle \} + U \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} = U \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \end{aligned} \quad (24)$$

We get the following matrix

$$\begin{array}{c} \frac{|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle}{\sqrt{2}} \\ \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \end{array} \begin{pmatrix} \frac{|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle}{\sqrt{2}} & \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \\ 0 & 0 \\ 0 & U \end{pmatrix} \quad (25)$$

As it appears, the subspace is already diagonal in the eigenbasis of  $\hat{P}$ . The  $\hat{P} = 1$  eigenstates are eigenstates of  $\mathcal{H}$ , with eigenvalues 0 and  $U$ . Next I look at the eigenstates of  $\hat{P} = -1$ .

$$\begin{aligned}
\mathcal{H} \frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}} \left\{ \left( c_{1\downarrow}^\dagger c_{2\downarrow} c_{2\uparrow}^\dagger c_{1\uparrow} \right) |\uparrow, \downarrow\rangle - \left( c_{1\uparrow}^\dagger c_{2\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow} \right) |\downarrow, \uparrow\rangle \right\} \\
&= -\frac{t}{\sqrt{2}} \{ |\downarrow\uparrow, 0\rangle + |0, \uparrow\downarrow\rangle - |\uparrow\downarrow, 0\rangle - |0, \downarrow\uparrow\rangle \} \\
&= 2t \frac{|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle}{\sqrt{2}} \\
\mathcal{H} \frac{|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}} \left\{ \left( c_{2\uparrow}^\dagger c_{1\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow} \right) |\uparrow\downarrow, 0\rangle - \left( c_{1\uparrow}^\dagger c_{2\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow} \right) |0, \uparrow\downarrow\rangle \right\} + U \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \\
&= -\frac{t}{\sqrt{2}} \{ |\downarrow, \uparrow\rangle - |\uparrow, \downarrow\rangle - |\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle \} + U \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \\
&= 2t \frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{2} + U \frac{|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle}{\sqrt{2}}
\end{aligned} \tag{26}$$

$$\begin{array}{c}
\frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}} \quad \frac{|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle}{\sqrt{2}} \\
\frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}} \left( \begin{array}{cc} 0 & 2t \\ 2t & U \end{array} \right) \\
\frac{|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle}{\sqrt{2}}
\end{array} \tag{27}$$

This subspace is not automatically diagonal, but is easily diagonalized. The eigenvectors are

$$\begin{aligned}
&\frac{1}{N_{\pm}} \left\{ 2t \frac{(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle)}{\sqrt{2}} + \frac{U \pm \sqrt{U^2 + 16t^2}}{2} \frac{(|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle)}{\sqrt{2}} \right\} \\
N_{\pm} &= \left\{ \frac{U}{2} \left[ U \pm \sqrt{U^2 + 16t^2} \right] + 16t^2 \right\}^{\frac{1}{2}}
\end{aligned} \tag{28}$$

with eigenvalues  $\frac{U \pm \sqrt{U^2 + 16t^2}}{2}$  respectively.

## 1.7 The total spectrum

| $\hat{N}$ | $S_z^{tot}$ | $\hat{P}$ | $\mathcal{H}$                  |   |
|-----------|-------------|-----------|--------------------------------|---|
| 1         | -1          | 1         | -t                             | $\frac{ \downarrow,0\rangle+ 0,\downarrow\rangle}{\sqrt{2}}$  |
|           |             | -1        | t                              | $\frac{ \downarrow,0\rangle- 0,\downarrow\rangle}{\sqrt{2}}$  |
|           | 1           | 1         | -t                             | $\frac{ \uparrow,0\rangle+ 0,\uparrow\rangle}{\sqrt{2}}$  |
|           |             | -1        | t                              | $\frac{ \uparrow,0\rangle- 0,\uparrow\rangle}{\sqrt{2}}$  |
| 2         | -1          | 1         | 0                              | $ \downarrow,\downarrow\rangle$   |
|           | 0           | 1         | 0                              | $\frac{ \uparrow,\downarrow\rangle+ \downarrow,\uparrow\rangle}{\sqrt{2}}$  |
|           |             | 1         | U                              | $\frac{ \uparrow\downarrow,0\rangle+ 0,\uparrow\downarrow\rangle}{\sqrt{2}}$  |
|           |             | -1        | $\frac{U+\sqrt{U^2+16t^2}}{2}$ | $\frac{1}{N_{\pm}}\left\{2t\frac{( \uparrow,\downarrow\rangle- \downarrow,\uparrow\rangle)}{\sqrt{2}}+\frac{U\pm\sqrt{U^2+16t^2}}{2}\frac{( \uparrow\downarrow,0\rangle- 0,\uparrow\downarrow\rangle)}{\sqrt{2}}\right\}$ |
|           |             | -1        | $\frac{U-\sqrt{U^2+16t^2}}{2}$ | $\frac{1}{N_{-}}\left\{2t\frac{( \uparrow,\downarrow\rangle- \downarrow,\uparrow\rangle)}{\sqrt{2}}+\frac{U-\sqrt{U^2+16t^2}}{2}\frac{( \uparrow\downarrow,0\rangle- 0,\uparrow\downarrow\rangle)}{\sqrt{2}}\right\}$     |
|           |             | 1         | 1                              | 0   |
|           | -1          | 1         | U-t                            | $\frac{ \uparrow\downarrow,\downarrow\rangle+ \downarrow,\uparrow\downarrow\rangle}{\sqrt{2}}$  |
| 3         | -1          | -1        | U+t                            | $\frac{ \uparrow\downarrow,\downarrow\rangle- \downarrow,\uparrow\downarrow\rangle}{\sqrt{2}}$  |
|           | 1           | 1         | U-t                            | $\frac{ \uparrow\downarrow,\uparrow\rangle+ \uparrow,\uparrow\downarrow\rangle}{\sqrt{2}}$  |
|           |             | -1        | U+t                            | $\frac{ \uparrow\downarrow,\uparrow\rangle- \uparrow,\uparrow\downarrow\rangle}{\sqrt{2}}$  |
| 4         | 0           | 1         | 2U                             | $ \uparrow\downarrow,\uparrow\downarrow\rangle$   |