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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. μ is the chemical potential, $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are the fermionic creation and annihilation operators at the i^{th} site, with spin-index σ . σ 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^{th} site and at spin-index σ ; 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:** $[\mathcal{H}, \hat{N}] = 0$. 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.
- $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$:

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

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

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:** $\hat{S}_{tot}^z \equiv \frac{1}{2} \sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$, $[\mathcal{H}, \hat{S}_{tot}^z] = 0$. 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 $[\mathcal{H}, \sum_i \hat{n}_{i\downarrow}]$. From eq. 2,

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

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

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 α and β ,

$$\hat{P} |\Psi(\alpha, \beta)\rangle = |\Psi(\beta, \alpha)\rangle \tag{6}$$

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

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

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,

$$\begin{aligned}\hat{P}\mathcal{H}|\Phi(\alpha, \beta)\rangle &= E(\alpha, \beta)\hat{P}|\Phi(\alpha, \beta)\rangle = E(\beta, \alpha)|\Phi(\beta, \alpha)\rangle \\ &= \mathcal{H}|\Phi(\beta, \alpha)\rangle = \mathcal{H}\hat{P}|\Phi(\alpha, \beta)\rangle \\ \implies \mathcal{H}\hat{P}|\Phi(\alpha, \beta)\rangle &= \hat{P}\mathcal{H}|\Phi(\alpha, \beta)\rangle\end{aligned}\tag{8}$$

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 $|\Psi(\alpha, \beta)\rangle$:

$$\mathcal{H}\hat{P}|\Psi(\alpha, \beta)\rangle = \hat{P}\mathcal{H}|\Psi(\alpha, \beta)\rangle \implies [\mathcal{H}, \hat{P}] = 0\tag{9}$$

1.2 Partitioning the Hilbert space

The Hamiltonian commutes with the three operators. This means that is possible to simultaneously diagonalize these four operators: $\mathcal{H}, \hat{N}, S_z^{tot}, \hat{P}$. 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 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 μN , 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 $S_z^{tot} = -1$.

$$\begin{aligned}\mathcal{H}|\downarrow, 0\rangle &= -tc_{2\downarrow}^\dagger c_{1\downarrow}|\downarrow, 0\rangle = -t|0, \downarrow\rangle \\ \mathcal{H}|0, \downarrow\rangle &= -tc_{1\downarrow}^\dagger c_{2\downarrow}|0, \downarrow\rangle = -t|\downarrow, 0\rangle\end{aligned}\tag{10}$$

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

$$\begin{array}{cc} & \begin{array}{cc} |\downarrow, 0\rangle & |0, \downarrow\rangle \end{array} \\ \begin{array}{c} |\downarrow, 0\rangle \\ |0, \downarrow\rangle \end{array} & \begin{pmatrix} 0 & -t \\ -t & 0 \end{pmatrix} \end{array}\tag{11}$$

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.

$$\begin{aligned}\hat{P}(|\downarrow, 0\rangle + |0, \downarrow\rangle) &= |0, \downarrow\rangle + |\downarrow, 0\rangle \implies \hat{P} = 1 \\ \hat{P}(|\downarrow, 0\rangle - |0, \downarrow\rangle) &= |0, \downarrow\rangle - |\downarrow, 0\rangle \implies \hat{P} = -1\end{aligned}\tag{12}$$

1.3.2 $S_z^{tot} = +1$

Now I look at the spin-up states.

$$\begin{aligned}\mathcal{H}|\uparrow, 0\rangle &= -tc_{2\uparrow}^\dagger c_{1\uparrow}|\uparrow, 0\rangle = -t|0, \uparrow\rangle \\ \mathcal{H}|0, \uparrow\rangle &= -tc_{1\uparrow}^\dagger c_{2\uparrow}|0, \uparrow\rangle = -t|\uparrow, 0\rangle\end{aligned}\tag{13}$$

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

$$\begin{array}{cc} & \begin{array}{cc} |\uparrow, 0\rangle & |0, \uparrow\rangle \end{array} \\ \begin{array}{c} |\uparrow, 0\rangle \\ |0, \uparrow\rangle \end{array} & \begin{pmatrix} 0 & -t \\ -t & 0 \end{pmatrix} \end{array}\tag{14}$$

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 $S_z^{tot} = -1$

$$\begin{aligned}\mathcal{H}|\uparrow\downarrow, \downarrow\rangle &= -tc_{2\uparrow}^\dagger c_{1\uparrow}|\uparrow\downarrow, \downarrow\rangle + U|\uparrow\downarrow, \downarrow\rangle = -t|\downarrow, \uparrow\downarrow\rangle + U|\uparrow\downarrow, \downarrow\rangle \\ \mathcal{H}|\downarrow, \uparrow\downarrow\rangle &= -tc_{1\uparrow}^\dagger c_{2\uparrow}|\downarrow, \uparrow\downarrow\rangle + U|\downarrow, \uparrow\downarrow\rangle = -t|\uparrow\downarrow, \downarrow\rangle + U|\downarrow, \uparrow\downarrow\rangle\end{aligned}\quad (15)$$

$$\begin{array}{c} |\uparrow\downarrow, \downarrow\rangle \quad |\downarrow, \uparrow\downarrow\rangle \\ |\uparrow\downarrow, \downarrow\rangle \left(\begin{array}{cc} U & -t \\ -t & U \end{array} \right) \\ |\downarrow, \uparrow\downarrow\rangle \end{array} \quad (16)$$

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 $S_z^{tot} = +1$

$$\begin{aligned}\mathcal{H}|\uparrow\downarrow, \uparrow\rangle &= -tc_{2\downarrow}^\dagger c_{1\downarrow}|\uparrow\downarrow, \uparrow\rangle + U|\uparrow\downarrow, \uparrow\rangle = tc_{2\downarrow}^\dagger c_{1\downarrow}|\downarrow\uparrow, \uparrow\rangle + U|\uparrow\downarrow, \uparrow\rangle \\ &= t|\uparrow, \downarrow\uparrow\rangle + U|\uparrow\downarrow, \uparrow\rangle = -t|\uparrow, \uparrow\downarrow\rangle + U|\uparrow\downarrow, \uparrow\rangle \\ \mathcal{H}|\uparrow, \uparrow\downarrow\rangle &= -tc_{1\downarrow}^\dagger c_{2\downarrow}|\uparrow, \uparrow\downarrow\rangle + U|\uparrow, \uparrow\downarrow\rangle = tc_{1\downarrow}^\dagger c_{2\downarrow}|\uparrow, \downarrow\uparrow\rangle + U|\uparrow, \uparrow\downarrow\rangle \\ &= t|\downarrow\uparrow, \uparrow\rangle + U|\uparrow, \uparrow\downarrow\rangle = -t|\uparrow\downarrow, \uparrow\rangle + U|\uparrow, \uparrow\downarrow\rangle\end{aligned}\quad (17)$$

$$\begin{array}{c} |\uparrow\downarrow, \uparrow\rangle \quad |\uparrow, \uparrow\downarrow\rangle \\ |\uparrow\downarrow, \uparrow\rangle \left(\begin{array}{cc} U & -t \\ -t & U \end{array} \right) \\ |\uparrow, \uparrow\downarrow\rangle \end{array} \quad (18)$$

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,

$$\mathcal{H}|\uparrow\downarrow, \uparrow\downarrow\rangle = 2U|\uparrow\downarrow, \uparrow\downarrow\rangle \quad (19)$$

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

$$\mathcal{H}|\downarrow, \downarrow\rangle = \mathcal{H}|\uparrow, \uparrow\rangle = 0 \quad (20)$$

1.6.2 $S_z^{tot} = 0$

This subspace has four eigenvectors,

$$|\uparrow, \downarrow\rangle, \quad |\downarrow, \uparrow\rangle, \quad |0, \uparrow\downarrow\rangle, \quad |\uparrow\downarrow, 0\rangle \quad (21)$$

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

$$\begin{aligned} \hat{P}(|\uparrow, \downarrow\rangle \pm |\downarrow, \uparrow\rangle) &= \pm(|\uparrow, \downarrow\rangle \pm |\downarrow, \uparrow\rangle) \\ \hat{P}(|\uparrow\downarrow, 0\rangle \pm |0, \uparrow\downarrow\rangle) &= \pm(|\uparrow\downarrow, 0\rangle \pm |0, \uparrow\downarrow\rangle) \end{aligned} \quad (22)$$

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.

$$\begin{aligned} \mathcal{H} \frac{|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}} \left\{ \left(c_{1\downarrow}^\dagger c_{2\downarrow} + c_{2\uparrow}^\dagger c_{1\uparrow} \right) |\uparrow, \downarrow\rangle + \left(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow} \right) |\downarrow, \uparrow\rangle \right\} \\ &= -\frac{t}{\sqrt{2}} \{ |\downarrow\uparrow, 0\rangle + |0, \uparrow\downarrow\rangle + |\uparrow\downarrow, 0\rangle + |0, \downarrow\uparrow\rangle \} = 0 \\ \mathcal{H} \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}} \left\{ \left(c_{2\uparrow}^\dagger c_{1\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow} \right) |\uparrow\downarrow, 0\rangle + \left(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow} \right) |0, \uparrow\downarrow\rangle \right\} + U \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \\ &= -\frac{t}{\sqrt{2}} \{ |\downarrow, \uparrow\rangle - |\uparrow, \downarrow\rangle + |\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle \} + U \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} = U \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \end{aligned} \quad (23)$$

We get the following matrix

$$\begin{array}{c} \frac{|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle}{\sqrt{2}} \\ \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \end{array} \begin{pmatrix} \frac{|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle}{\sqrt{2}} & \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \\ 0 & 0 \\ 0 & U \end{pmatrix} \quad (24)$$

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 $\hat{P} = -1$.

$$\begin{aligned} \mathcal{H} \frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}} \left\{ \left(c_{1\downarrow}^\dagger c_{2\downarrow} c_{2\uparrow}^\dagger c_{1\uparrow} \right) |\uparrow, \downarrow\rangle - \left(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow} \right) |\downarrow, \uparrow\rangle \right\} \\ &= -\frac{t}{\sqrt{2}} \{ |\downarrow\uparrow, 0\rangle + |0, \uparrow\downarrow\rangle - |\uparrow\downarrow, 0\rangle - |0, \downarrow\uparrow\rangle \} \\ &= 2t \frac{|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle}{\sqrt{2}} \\ \mathcal{H} \frac{|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}} \left\{ \left(c_{2\uparrow}^\dagger c_{1\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow} \right) |\uparrow\downarrow, 0\rangle - \left(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow} \right) |0, \uparrow\downarrow\rangle \right\} + U \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \\ &= -\frac{t}{\sqrt{2}} \{ |\downarrow, \uparrow\rangle - |\uparrow, \downarrow\rangle - |\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle \} + U \frac{|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{\sqrt{2}} \\ &= 2t \frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{2} + U \frac{|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle}{\sqrt{2}} \end{aligned} \quad (25)$$

$$\begin{array}{c} \frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}} \\ \frac{|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle}{\sqrt{2}} \end{array} \begin{pmatrix} \frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}} & \frac{|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle}{\sqrt{2}} \\ 0 & 2t \\ 2t & U \end{pmatrix} \quad (26)$$

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

$$\begin{aligned} \frac{1}{N_\pm} \left\{ 2t \frac{(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle)}{\sqrt{2}} + \frac{U \pm \sqrt{U^2 + 16t^2}}{2} \frac{(|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle)}{\sqrt{2}} \right\} \\ N_\pm = \left\{ \frac{U}{2} \left[U \pm \sqrt{U^2 + 16t^2} \right] + 16t^2 \right\}^{\frac{1}{2}} \end{aligned} \quad (27)$$

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

1.7 The total spectrum

\hat{N}	S_z^{tot}	\hat{P}	E	$ \Phi\rangle$
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	0	-1	1	$ \downarrow, \downarrow\rangle$
			1	$\frac{ \uparrow,\downarrow\rangle+ \downarrow,\uparrow\rangle}{\sqrt{2}}$
		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	$ \uparrow, \uparrow\rangle$
3	-1	1	U-t	$\frac{ \uparrow\downarrow,\downarrow\rangle+ \downarrow,\uparrow\downarrow\rangle}{\sqrt{2}}$
		-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$