....

....

(......................)

....

1 Exact diagonalization of the two-site Hubbard model

The Hamiltonian

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

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 ith 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 ith 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**: $\left[\mathcal{H}, \hat{N} \right] = 0$. 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.

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

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

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

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

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

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

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

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

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

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

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

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

Finally, $[N, \hat{n}_{i\downarrow}] = \sum_{j\sigma} [\hat{n}_{j\sigma}, \hat{n}_{i\downarrow}] = [\hat{n}_{i\uparrow}, \hat{n}_{i\downarrow}] = c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} - c^\dagger_{i\downarrow} c_{i\downarrow} c^\dagger_{i\uparrow} c_{i\uparrow} = 0$. Since $\hat{S}^z_{tot}$ 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 it's site indices. I now rewrite the Hamiltonian by explcitly showing the two site indices:

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

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,

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

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: $\mathcal{H}, \hat{N}, S^{tot}_z, \hat{P}$. I will be able to label the eigenstates of the total Hamiltonian using the eigenvalues of these operatos. 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^{tot}_z. 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: $\mathcal{H} \to \mathcal{H} + \mu\hat{N} = -t \sum_\sigma \left(c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$. This will keep the eigenvectors unaltered, but will increase the eigenvalues by μN, where N is the number of particles in the eigenstate I am 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 $S_z^{tot} = -1$.

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

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.

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

1.3.2 $S_z^{tot} = +1$

Now I look at the spin-up states.

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

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 $S_z^{tot} = -1$

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

$$
\begin{array}{c}
\quad\quad |\uparrow\downarrow, \downarrow\rangle \quad |\downarrow, \uparrow\downarrow\rangle \\
\begin{array}{c} |\uparrow\downarrow, \downarrow\rangle \\ \\ |\downarrow, \uparrow\downarrow\rangle \end{array}
\begin{pmatrix} U & -t \\ \\ -t & U \end{pmatrix}
\end{array}
\tag{16}
$$

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 $S_z^{tot} = +1$

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

$$
\begin{array}{c}
\quad\quad |\uparrow\downarrow, \uparrow\rangle \quad |\uparrow, \uparrow\downarrow\rangle \\
\begin{array}{c} |\uparrow\downarrow, \uparrow\rangle \\ \\ |\uparrow, \uparrow\downarrow\rangle \end{array}
\begin{pmatrix} U & -t \\ \\ -t & U \end{pmatrix}
\end{array}
\tag{18}
$$

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,

$$
\mathcal{H} |\uparrow\downarrow, \uparrow\downarrow\rangle = 2U |\uparrow\downarrow, \uparrow\downarrow\rangle
\tag{19}
$$

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 theya 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

$$\mathcal{H}\left|\downarrow,\downarrow\right\rangle = \mathcal{H}\left|\uparrow,\uparrow\right\rangle = 0 \tag{20}$$

1.6.2 $S_z^{tot} = 0$

This subspace has four eigenvectors,

$$\left|\uparrow,\downarrow\right\rangle, \qquad \left|\downarrow,\uparrow\right\rangle, \qquad \left|0,\uparrow\downarrow\right\rangle, \qquad \left|\uparrow\downarrow,0\right\rangle \tag{21}$$

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

$$\hat{P}\left(\left|\uparrow,\downarrow\right\rangle \pm \left|\downarrow,\uparrow\right\rangle\right) = \pm\left(\left|\uparrow,\downarrow\right\rangle \pm \left|\downarrow,\uparrow\right\rangle\right)$$
$$\hat{P}\left(\left|\uparrow\downarrow,0\right\rangle \pm \left|0,\uparrow\downarrow\right\rangle\right) = \pm\left(\left|\uparrow\downarrow,0\right\rangle \pm \left|0,\uparrow\downarrow\right\rangle\right) \tag{22}$$

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

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

- $\hat{P} = -1 : \frac{\left|\uparrow,\downarrow\right\rangle - \left|\downarrow,\uparrow\right\rangle}{\sqrt{2}}, \qquad \frac{\left|\uparrow\downarrow,0\right\rangle - \left|0,\uparrow\downarrow\right\rangle}{\sqrt{2}}$

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.

$$\mathcal{H}\frac{\left|\uparrow,\downarrow\right\rangle + \left|\downarrow,\uparrow\right\rangle}{\sqrt{2}} = -\frac{t}{\sqrt{2}}\left\{\left(c_{1\downarrow}^{\dagger}c_{2\downarrow} + c_{2\uparrow}^{\dagger}c_{1\uparrow}\right)\left|\uparrow,\downarrow\right\rangle + \left(c_{1\uparrow}^{\dagger}c_{2\uparrow} + c_{2\downarrow}^{\dagger}c_{1\downarrow}\right)\left|\downarrow,\uparrow\right\rangle\right\}$$

$$= -\frac{t}{\sqrt{2}}\left\{\left|\downarrow\uparrow,0\right\rangle + \left|0,\uparrow\downarrow\right\rangle + \left|\uparrow\downarrow,0\right\rangle + \left|0,\downarrow\uparrow\right\rangle\right\} = 0$$

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

$$= -\frac{t}{\sqrt{2}}\left\{\left|\downarrow,\uparrow\right\rangle - \left|\uparrow,\downarrow\right\rangle + \left|\uparrow,\downarrow\right\rangle - \left|\downarrow,\uparrow\right\rangle\right\} + U\frac{\left|\uparrow\downarrow,0\right\rangle + \left|0,\uparrow\downarrow\right\rangle}{\sqrt{2}} = U\frac{\left|\uparrow\downarrow,0\right\rangle + \left|0,\uparrow\downarrow\right\rangle}{\sqrt{2}}$$

We get the following matrix

$$\begin{array}{cc} & \begin{array}{cc} \frac{\left|\uparrow,\downarrow\right\rangle + \left|\downarrow,\uparrow\right\rangle}{\sqrt{2}} & \frac{\left|\uparrow\downarrow,0\right\rangle + \left|0,\uparrow\downarrow\right\rangle}{\sqrt{2}} \end{array} \\ \begin{array}{c} \frac{\left|\uparrow,\downarrow\right\rangle + \left|\downarrow,\uparrow\right\rangle}{\sqrt{2}} \\ \frac{\left|\uparrow\downarrow,0\right\rangle + \left|0,\uparrow\downarrow\right\rangle}{\sqrt{2}} \end{array} & \begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix} \end{array} \tag{24}$$

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 $\hat{P} = -1$.

$$\mathcal{H}\,\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}} = -\frac{t}{\sqrt{2}}\left\{\left(c_{1\downarrow}^{\dagger}c_{2\downarrow}c_{2\uparrow}^{\dagger}c_{1\uparrow}\right)|\uparrow,\downarrow\rangle - \left(c_{1\uparrow}^{\dagger}c_{2\uparrow} + c_{2\downarrow}^{\dagger}c_{1\downarrow}\right)|\downarrow,\uparrow\rangle\right\}$$

$$= -\frac{t}{\sqrt{2}}\left\{|\downarrow\uparrow,0\rangle + |0,\uparrow\downarrow\rangle - |\uparrow\downarrow,0\rangle - |0,\downarrow\uparrow\rangle\right\}$$

$$= 2t\,\frac{|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle}{\sqrt{2}}$$

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

$$= -\frac{t}{\sqrt{2}}\left\{|\downarrow,\uparrow\rangle - |\uparrow,\downarrow\rangle - |\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\right\} + U\,\frac{|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle}{\sqrt{2}}$$

$$= 2t\,\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{2} + U\,\frac{|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle}{\sqrt{2}}$$

$$(25)$$

$$\begin{array}{c} \\ \frac{|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle}{\sqrt{2}} \\[1em] \frac{|\uparrow\downarrow,0\rangle-|0,\uparrow\downarrow\rangle}{\sqrt{2}} \end{array} \begin{array}{cc} \frac{|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle}{\sqrt{2}} & \frac{|\uparrow\downarrow,0\rangle-|0,\uparrow\downarrow\rangle}{\sqrt{2}} \\ \left(\begin{array}{cc} 0 & 2t \\[1.5em] 2t & U \end{array}\right) \end{array} \qquad (26)$$

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

$$\frac{1}{N_{\pm}}\left\{2t\,\frac{(|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle)}{\sqrt{2}} + \frac{U \pm \sqrt{U^2+16t^2}}{2}\,\frac{(|\uparrow\downarrow,0\rangle-|0,\uparrow\downarrow\rangle)}{\sqrt{2}}\right\}$$

$$N_{\pm} = \left\{\frac{U}{2}\left[U \pm \sqrt{U^2+16t^2}\right] + 16t^2\right\}^{\frac{1}{2}}$$

$$(27)$$

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

1.7 The total spectrum

The final spectrum is already obtained. One final thing to do is to just add the respective values of $-\mu N$ to the eigenvalues.

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